On three-dimensional spiral anisotropic self-avoiding walks

1985 J. Phys. A: Math. Gen. 18 L1049

(http://iopscience.iop.org/0305-4470/18/16/010)

J. Phys. A: Math. Gen. 18 (1985) L1049–L1054. Printed in Great Britain

LETTER TO THE EDITOR

On three-dimensional spiral anisotropic self-avoiding walks

A J Guttmann and K J Wallace

Department of Mathematics, Statistics and Computer Science, The University of Newcastle, NSW 2308, Australia

Received 9 August 1985

Abstract. Two new models of three-dimensional anisotropic spiral self-avoiding walks are introduced with different types of spiral constraint. Series expansions for the two models are derived and analysed. One model is found to behave like the isotropic three-dimensional self-avoiding walk, while the other model appears to belong to a distinct universality class, with exponents $\nu \approx 0.655$ and $\gamma \approx 1.24$. It is argued that for these non-Markovian, undirected, unweighted walks, the absence of a plane of reflection symmetry in the allowed walks signals a new universality class.

Recently a variety of anistropic two-dimensional self-avoiding walks have been shown to have different critical exponents from that of ordinary (isotropic) SAWS. For ordinary SAWS, the two most frequently encountered exponents are γ and ν, defined by

$$C(x) = \sum_{n \geq 0} c_n x^n \sim A(1-\mu x)^{-\gamma}$$

$$\langle R_n^2 \rangle \sim Bn^{2\nu}, \tag{1}$$

where c_n is the number of distinct n-step walks with a common origin, $C(x)$ is thus their generating function, μ is a (lattice dependent) constant called the connective constant and $\langle R_n^2 \rangle$ is the mean square end-to-end distance of an n-step walk, averaged over all c_n such walks. For the two-dimensional SAW, Nienhius (1982, 1984) has shown (non-rigorously) that $\gamma = 43/32$ and $\nu = 3/4$.

The anisotropic walks referred to above include spiral self-avoiding walks on the square lattice (Privman 1983) whose dominant critical behaviour (Blöte and Hilhorst 1984, Guttmann and Wormald 1984) was found to be completely different from that of SAWS, in that

$$c_n \sim C \exp[2\pi(n/3)^{1/2}]/n^{7/4}$$

$$\langle R_n^2 \rangle \sim Dn \log(n) \tag{2}$$

so that $\nu = \frac{1}{2}$ (with a confluent logarithmic term) and γ is undefined. Manna (1984) recently introduced spiral anisotropic walks in which the spiral constraint is applied to steps along only one of the two orthogonal lattice axes. The behaviour of such walks appears to be (Guttmann and Wallace 1985)

$$c_n \sim E\mu^n \exp(\alpha\sqrt{n}) n^{\beta}$$

$$\langle R_n^2 \rangle \sim Fn^{2\nu} \tag{3}$$

with $\nu \approx 0.855$, and with μ known exactly (Whittington 1985) and $\beta \approx 0.9$.

In this letter we study two three-dimensional anisotropic spiral SAWs in an attempt to see whether this unusual critical behaviour (2) and (3) above carries over into three dimensions and, more importantly, in order to determine which geometrical features of a SAW model control its critical behaviour.

One model we have considered is a pure spiral self-avoiding walk, defined as a self-avoiding walk on the simple cubic lattice in which no step through an angle of $-\pi/2$ may be made. Thus the number of choices that may be made at each vertex is at most three: straight ahead, a turn through $\pi/2$ on one orthogonal axis, or a turn through $\pi/2$ on the other. This model is clearly a three-dimensional generalisation of the square lattice spiral SAW introduced by Privman (1983). We will refer to this model as model S (for spiral). The second model retains the usual simple cubic lattice choices in four of the six axes, but steps along the z axis are constrained by the following rule: steps in the $+z$ direction can only be followed by steps in the $+z$ or $+y$ directions, while steps in the $-z$ direction can only be followed by steps in the $-z$ or $-y$ directions. This model, which we refer to as model A (for anisotropic) is a three-dimensional generalisation of Manna's anisotropic spiral SAWs, in that it has the spiral constraint applied to steps in one lattice direction only.

We have generated series expansions for both models, calculating c_n and $\langle R_n^2\rangle$ up to $n=18$ for model A and up $n=23$ for model S. The programs used an efficient backtracking algorithm, essentially comprising of nested do-loops that generated the walks in pre-order sequence, thus minimising storage requirements, in that only the current walk needs to be stored. Maximum use of symmetry was also invoked. The

Table 1. Series coefficients of the two models.

	Spiral walks (Model S)			Anisotropic walks (Model A)		
n	c_n	p_n	$\langle R_n^2\rangle$	c_n	p_n	$\langle R_n^2\rangle$
1	6	6	1.000 0000	6	6	1.000 0000
2	18	48	2.666 6667	24	60	2.500 0000
3	54	222	4.111 1111	90	378	4.222 0000
4	150	840	5.600 0000	324	1 992	6.148 1481
5	426	2 922	6.859 1549	1 166	9 518	8.162 9503
6	1 158	9 816	8.476 6839	4 138	42 832	10.350 8942
7	3 204	32 268	10.071 1610	14 730	184 866	12.550 3055
8	8 682	103 920	11.969 5923	51 992	774 320	14.893 0605
9	23 724	327 972	13.824 4815	183 898	3 169 250	17.233 7383
10	64 194	1 016 604	15.836 4333	646 980	12 741 260	19.693 4372
11	174 378	3 104 886	17.805 4915	2 279 702	50 482 038	22.144 1390
12	470 856	9 372 384	19.904 9901	8 002 976	197 655 176	24.697 7095
13	1 274 430	28 021 722	21.987 6509	28 127 418	766 180 706	27.239 6388
14	3 434 826	83 102 064	24.193 9662	98 585 096	2 945 067 020	29.873 3494
15	9 272 346	244 684 278	26.388 6052	345 848 306	11 238 074 498	32.494 2303
16	24 953 004	715 869 972	28.688 7291	1 210 704 274	42 614 594 360	35.198 1861
17	67 230 288	2 082 493 224	30.975 5214	4 241 348 770	160 700 082 706	37.888 9102
18	180 705 126	6 027 558 060	33.355 7669	14 833 284 544	603 058 215 404	40.655 7438
19	486 152 604	17 367 361 116	35.724 0936			
20	1 305 430 884	49 839 214 272	38.178 3631			
21	3 507 947 838	142 499 394 102	40.621 8680			
22	9 412 114 986	406 078 307 556	43.144 2145			
23	25 268 587 338	1153 665 098 214	45.656 0979			

programs were run on a VAX 11/780, and used about 150 h and 130 h of CPU time for model A and model S respectively.

The series obtained were for $C(x)$, the sum over all c_n n-step SAWs square end-to-end distances r_n^2, $R(x)=\Sigma\rho_n x^n$, where $\rho_n=\Sigma r_n^2$, and the mean square end-to-end distance $\langle R_n^2\rangle=\rho_n/c_n$. These series are shown in table 1.

A brief analysis of the data indicated that it was amenable to analysis by standard methods, but that the anisotropic nature of the model has slow convergence compared to the isotropic SAW model.

The method of analysis of $C(x)$ and $R(x)$ upon which we placed the greatest reliance was the method of integral approximants, introduced by Guttmann and Joyce (1972) as the recurrence relation method. We utilised first- and second-order inhomogeneous integral approximants, with the degree of the inhomogeneous polynomial varying from 1 to 6.

First-order inhomogeneous approximants can successfully mimic an algebraic singularity plus an additive analytic background term, while second-order inhomogeneous approximants can mimic an algebraic singularity, a confluent singularity and an additive analytic background term.

The results of this analysis for both models are shown in table 2. The results are obtained from arithmetic means of all estimates obtained, with outsiders neglected, and the quoted error is $\pm 2\sigma$, where σ is the standard deviation of each mean. Experience with other lattice models leads us to believe that this is a conservative measure of the errors.

For model A, a combination of the results obtained from both first- and second-order approximants allows us to estimate

$$\mu^{-1}=0.2883\pm 0.0002$$
$$\gamma=1.16\pm 0.02 \qquad (4)$$
$$\gamma+2\nu=2.35\pm 0.03$$

hence

$$\nu=0.595\pm 0.025,$$

while for model S the series are less well converged and only allow us to estimate

$$\mu^{-1}=0.3765\pm 0.0002$$
$$\gamma=1.24\pm 0.2 \qquad (5)$$
$$\gamma+2\nu=2.58\pm 0.2$$

Table 2. Analysis of critical parameters of $C(x)$ and $R(x)$ series by first- and second-order inhomogeneous integral approximants.

		First-order integral approximants		Second-order integral approximants	
	Series	μ^{-1}	exponent	μ^{-1}	exponent
Model S	$C(x)$	0.3763 ± 0.0015	1.23 ± 0.13	0.3764 ± 0.0021	1.25 ± 0.20
	$R(x)$	0.3766 ± 0.0013	2.56 ± 0.12	0.3768 ± 0.0019	2.60 ± 0.26
Model A	$C(x)$	$0.288\,31\pm 0.000\,25$	1.163 ± 0.026	$0.288\,24\pm 0.000\,28$	1.154 ± 0.029
	$R(x)$	$0.288\,31\pm 0.000\,17$	2.347 ± 0.036	$0.288\,38\pm 0.000\,17$	2.354 ± 0.021

hence

$$\nu = 0.67 \pm 0.2.$$

Comparing the exponent estimates to the best renormalisation group (RG) estimates for the ordinary (isotropic) SAW (Le Guillou and Zinn-Justin 1980) of $\gamma = 1.1615 \pm 0.0020$ and $\nu = 0.5880 \pm 0.0015$, we see that the central exponent estimates for model A are quite close to the RG estimates, while for model S both ν and γ are rather higher, but with such wide error bounds as to readily include the RG estimates.

Turning to the $\langle R_n^2 \rangle$ series, we first analyse these by an elementary ratio-type method that does not take into account any confluent singularities. That is, we assume that

$$\langle R_n^2 \rangle \sim A n^{2\nu}(1 + c_1/n + c_2/n^2 + \cdots). \tag{6}$$

Estimates of ν are given by the sequences $\nu_n^{(1)}$, $\nu_n^{(2)}$, $\nu_n^{(3)}$ defined by

$$\begin{aligned} \nu_n^{(1)} &= \tfrac{1}{2}\ln(\langle R_n^2 \rangle / \langle R_{n-2}^2 \rangle)/\ln(n/(n-2)] \\ \nu_n^{(2)} &= [n\nu_n^{(1)} - (n-2)\nu_{n-2}^{(1)}]/2 \\ \nu_n^{(3)} &= [n^2\nu_n^{(2)} - (n-2)^2\nu_{n-2}^{(2)}]/(4n-4) \end{aligned} \tag{7}$$

where $\nu_n^{(2)}$ accounts for the first correction term in (6) and $\nu_n^{(3)}$ accounts for the next correction term. Alternate terms are used to minimise the effect of the loose-packed lattice structure. Averaging of the $\langle R_n^2 \rangle$ sequence in order to minimise the effect of a singularity on the negative real axis was also undertaken, with comparable results to those obtained from the above method. Padé approximants (not shown) also gave comparable estimates.

Table 3. Estimates of exponent ν by extrapolation.

	Model S			Model A		
n	$\nu_n^{(1)}$	$\nu_n^{(2)}$	$\nu_n^{(3)}$	$\nu_n^{(1)}$	$\nu_n^{(2)}$	$\nu_n^{(3)}$
10	0.627 27	0.737 53	0.510 56	0.626 03	0.600 82	0.598 36
11	0.630 55	0.632 05	0.214 39	0.624 66	0.596 47	0.585 22
12	0.627 07	0.626 06	0.372 72	0.620 95	0.595 54	0.583 52
13	0.631 45	0.636 43	0.647 46	0.619 86	0.593 44	0.585 79
14	0.632 93	0.668 07	0.784 41	0.617 11	0.594 08	0.590 05
15	0.637 49	0.676 74	0.798 38	0.616 31	0.593 24	0.592 66
16	0.638 06	0.673 95	0.693 12	0.614 19	0.593 75	0.592 68
17	0.640 22	0.660 72	0.604 39	0.613 58	0.593 12	0.592 69
18	0.639 85	0.654 18	0.579 77	0.611 91	0.593 67	0.593 35
19	0.641 17	0.649 17	0.602 81			
20	0.640 84	0.649 76	0.630 92			
21	0.641 87	0.648 57	0.645 86			
22	0.641 48	0.647 90	0.639 07			
23	0.642 13	0.644 81	0.625 95			

The results obtained are shown in table 3 for both models. For model A we estimate $\nu = 0.592 \pm 0.005$, while for model S we find $\nu = 0.645 \pm 0.015$. These results clearly suggest that model A has the same exponent as the isotropic SAW model, while model S is in a different universality class.

Now it can be argued that the correction terms assumed in (6) are almost certainly wrong, and that confluent terms are likely to be present. While this is true, it does not invalidate the above analysis. Rather, the presence of confluent terms will slow the apparent rate of convergence, and this is reflected in wider error bars.

An alternative method of analysis focuses on the question whether ν is the same as, or different from, the value of ν for isotropic SAWs by considering the exponent ϕ defined by

$$\langle R_n^2\rangle_X/\langle R_n^2\rangle_{\mathrm{SAW}} \sim Cn^{2\phi_X} \qquad (8)$$

where $\phi_X = \nu_X - \nu_{\mathrm{SAW}}$ for any model X.

For the SAW series on the simple cubic lattice, we have extended the series by four additional terms (to $n = 19$) (Guttmann 1985a) which allows us to form the quotient on the LHS of (8) for all coefficients for model A, and coefficients up to $n = 19$ for model S. Estimates of ϕ can be found from the sequences defined by (7), and these are shown in table 4.

For model A we see that linear extrapolants already suggest $|\phi| < 0.0036$, while quadratic extrapolants are smaller still. For model S the exponent estimates are *increasing*, suggesting $\phi > 0.039$, while linear extrapolants are less well behaved, nevertheless suggesting $\phi \leqslant 0.052$. These results reinforce our earlier conclusion that model A is in the same universality class as isotropic SAWs, while model S appears to be in a new, distinct universality class.

Table 4. Estimates of exponent ϕ as defined in equation (8).

	n	$\langle R_n^2\rangle_X/\langle R_n^2\rangle$	$\phi_n^{(1)}$	$\phi_n^{(2)}$	$\phi_n^{(3)}$
	7	0.924 194	−0.038 019	0.138 816	
	8	0.931 842	−0.005 004	0.261 186	
	9	0.935 314	0.023 796	0.240 145	
	10	0.941 678	0.023 528	0.137 653	
	11	0.945 021	0.025 725	0.034 409	
	12	0.949 990	0.024 099	0.026 959	
Model S	13	0.953 823	0.027 748	0.038 876	
	14	0.958 995	0.030 601	0.069 608	
	15	0.936 331	0.034 659	0.079 579	
	16	0.968 336	0.036 297	0.076 169	
	17	0.972 564	0.038 104	0.063 938	
	18	0.977 179	0.038 592	0.056 956	
	19	0.981 179	0.039 644	0.052 740	
	7	1.151 696	0.030 408	0.004 821	−0.039 643
	8	1.159 437	0.027 623	−0.001 815	−0.035 652
	9	1.165 972	0.024 510	0.003 864	0.002 398
	10	1.171 026	0.022 287	0.000 943	0.005 845
	11	1.175 293	0.019 840	−0.001 174	−0.011 375
Model A	12	1.178 728	0.017 978	−0.003 568	−0.013 820
	13	1.181 654	0.016 154	−0.004 117	−0.011 537
	14	1.184 113	0.014 783	−0.004 385	−0.006 648
	15	1.186 221	0.013 478	−0.003 916	−0.003 310
	16	1.188 051	0.012 432	−0.004 023	−0.002 840
	17	1.189 629	0.011 462	−0.003 657	−0.002 747
	18	1.191 037	0.010 656	−0.003 554	−0.001 787

If we ask why these two models differ in their universality class given that they are non-Markovian, non-directed and unweighted, a relevant observation seems to be that, if one considers all possible n-step walks, then there is a plane of reflection symmetry for model A walks and no plane of symmetry for model S walks. For model A walks, the yz plane is a plane of reflection symmetry. For both models there is at least one axis of rotational symmetry, but this appears unimportant. As we argue in Guttmann (1985b), the absence of a plane of reflection symmetry appears to signal a new universality class in all known cases in both two and three dimensions. These models then seem to fit this empirical observation. In two dimensions the spiral SAWs and Manhattan and L lattice SAWs (Guttmann 1983) are found to display behaviour supporting this hypothesis. The spiral SAWs have no axis of reflection symmetry and belong to a new universality class, while the Manhattan and L lattice SAWs appear to belong to the same universality class as the ordinary square lattice SAW, and do possess at least one axis of reflection symmetry.

In three dimensions the spiral constraint, as displayed in model S, is clearly weaker than its two-dimensional counterpart. This has the effect of producing a small ($\sim 10\%$) increase in the critical exponents ν and γ, while in two dimensions the functional form of $C(x)$ for spiral SAWs is quite different from its isotropic counterpart, with a growth term $\exp[2\pi(n/3)^{1/2}]$.

References

Blöte H W and Hilhorst H J 1984 *J. Phys. A: Math. Gen.* **17** L111
Guttmann A J 1983 *J. Phys. A: Math. Gen.* **16** 3885
—— 1985a in preparation
—— 1985b in preparation
Guttmann A J and Joyce G S 1972 *J. Phys. A: Gen. Phys.* **5** L81
Guttmann A J and Wallace K J 1985 submitted
Guttmann A J and Wormald N C 1984 *J. Phys. A: Math. Gen.* **17** L271
Le Guillou J C and Zinn-Justin J 1980 *Phys. Rev.* B **21** 3976
Manna S S 1984 *J. Phys. A: Math. Gen.* **17** L899
Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
—— 1984 *J. Stat. Phys.* **34** 731
Privman V 1983 *J. Phys. A: Math. Gen.* **16** L571
Whittington S G 1985 *J. Phys. A: Math. Gen.* **18** L67