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The shortest path of SAWs with bridges

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Abstract. The shortest paths of self-avoiding walks (SAWs) with bridge lengths $b = 1, \sqrt{2}, \sqrt{3}$ and 2 are studied by exact series expansions and by Monte Carlo simulation methods on the square and simple cubic lattices. In the series work, SAW configurations of up to 24 and 14 steps are generated on the square and simple cubic lattices respectively. Assuming the shortest path S_N between two sites, which are separated by N steps along the chain, has the scaling form $S_N \sim AN + BN^{1-\Delta}$, it is found that $\Delta = 1$ and $\Delta \simeq \frac{1}{2}$ on the square and simple cubic lattices respectively, independent of the bridge length. The problem is also investigated by the Mellin-Padé approximation method using Monte Carlo data on the square lattice. The latter method gives results consistent with those of the series expansion study. Our results are not consistent with earlier predictions.

1. Introduction

Self-avoiding walks (SAWs) continue to attract considerable research interest as model systems of both phase transitions and systems exhibiting interesting metric properties. A SAW configuration on the lattice is defined as a non-intersecting chain consisting of lattice sites connected by nearest-neighbour lattice bonds. It is generally accepted as a model for the study of the scaling properties of linear polymers in dilute solution [1]. In that model, the sites represent monomers and the bonds represent chemical bonds between monomer pairs. It is evident, however, that interactions are not confined only to these chemical bonds. Any two nearby monomers interact with each other. Hence, a better approximation to the real physical system is to connect pairs of sites in a SAW configuration with a weaker bond if the distance between them is within a certain range. These additional bonds are called 'bridges' by Helman *et al* [2]. They argued that the addition of bridges will change the scaling properties of the system. Subsequently, several authors studied different aspects of this 'SAWs with bridges' model [3], one of which is the shortest path [3-5].

The shortest path between two points is defined as the minimum number of bonds or bridges required to connect them. For ordinary SAWs, the shortest path is just the chain length between these two points. The addition of bridges creates 'short cuts' and the shortest path becomes shorter than the chain length. If we think of the system as a kind of 'blob and link' structure [3], that is, a finite fraction of the bonds still form a linear structure, then we expect S_N/N to approach a non-zero constant, where S_N is the average length of the shortest path with N monomers. However, the problem

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of the correction to leading order behaviour is still an open question. Earlier Monte Carlo simulations by Yang *et al* [3] suggested that the leading correction exponent in dimensionality $d = 2$–6 is superuniversal (independent of dimension). Subsequent work by Barat *et al* [4] claimed to find a similar result. However, we believe that the earlier work is not reliable because of an inappropriate method used to extract the exponent.

The present paper is aimed at an extensive study of the problem by both longer series for the series expansion study, and a greater number of configurations as well as larger configuration sizes for the Monte Carlo study.

2. Numerical simulations

The SAW configurations are generated by the conventional back-tracking algorithm on two- and three-dimensional hypercubic lattices of unit lattice spacing. Pairs of sites within a Euclidean distance b are considered to be connected. For each SAW configuration, one of the end sites is labelled as '0'. The sites of the walk which are connected to the site '0' are labelled '1', and the unlabelled sites of the walk which are connected to '1'-sites are labelled '2', etc. From the definition of the shortest path, the label of a site is equal to the shortest path from that site to the origin. All SAW configurations are generated and the end-to-end shortest path of each configuration is accumulated to give $S_N C_N$. Here C_N is the total number of SAWs of N bonds. The square lattice series and the simple cubic lattice series are tabulated in table 1 and table 2 respectively. Our $b = 1$ results for $N \leqslant 18$ on the square lattice and $N \leqslant 11$ on the simple cubic

Table 1. Series coefficients for the shortest path of SAWs on square lattice.

	$S_N C_N$		
N	$b = 1$	$b = \sqrt{2}$	$b = 2$
1	4	4	4
2	24	16	12
3	92	68	64
4	336	232	160
5	1 132	796	676
6	3 720	2 528	1 732
7	11 684	8 036	6 440
8	36 384	24 520	16 688
9	110 028	74 796	57 620
10	331 720	222 400	150 580
11	979 276	660 868	494 776
12	2 888 464	1 929 944	1 301 208
13	8 386 412	5 631 748	4 126 100
14	24 349 160	16 228 768	10 903 692
15	69 835 548	46 730 860	33 663 256
16	200 362 176	133 288 872	89 287 024
17	569 268 356	379 917 092	269 997 636
18	1 618 172 568	1 074 853 312	718 153 380
19	4 563 244 964	3 039 122 932	2 136 075 840
20	12 875 108 576	8 541 661 232	5 693 969 456
21	36 086 945 324	23 994 293 596	16 710 504 036
22	101 200 051 112	67 070 070 848	44 618 212 196
23	282 213 901 868	187 391 828 604	
24	787 411 392 176		

Table 2. Series coefficients for the shortest path of SAWs on simple cubic lattice.

	$S_N C_N$			
N	$b=1$	$b=\sqrt{2}$	$b=\sqrt{3}$	$b=2$
1	6	6	6	6
2	60	36	36	30
3	402	282	234	228
4	2 520	1 488	1 392	1 188
5	14 502	9 126	7 830	7 194
6	81 972	47 676	43 068	36 858
7	444 930	267 330	230 898	204 864
8	2 395 632	1 373 928	1 221 768	1 041 480
9	12 587 214	7 358 862	6 368 046	5 530 638
10	65 860 188	37 355 604	32 922 276	27 894 942
11	339 003 810	194 622 618	168 490 842	144 240 036
12	1 740 598 344	978 491 232	857 501 040	722 056 260
13	8 833 106 358	5 005 280 574	4 332 475 230	3 669 902 898
14	44 751 148 932	24 972 014 172		

lattice are consistent with previously known data [4, 5], though we have extended the square lattice and the simple cubic lattice series by six and three terms respectively.

To analyse the series data, we first assume a power law correction to leading order,

$$R_N \equiv \frac{S_N}{N} \sim A + BN^{-\Delta} \qquad N \to \infty. \tag{1}$$

The parameters A, B and Δ can then be determined by the following set of simultaneous equations:

$$R_{N-i} = A + B(N-i)^{-\Delta} \qquad i = 0, 2, 4. \tag{2}$$

Here we separate the even and odd N data to eliminate the oscillations characteristic of loose-packed lattices. The results for the square lattice and the simple cubic lattice are listed in table 3 for the best and worst cases, $b=1$ and $b=2$. Intermediate values of b give results which converged less rapidly than the case for $b=1$ and more rapidly than for $b=2$. We eliminated A and B from successive pairs of equations, resulting in a single, non-linear equation which we solved for Δ by the bisection method, and then calculated A and B by back substitution. We conclude from table 3 that $\Delta = 0.9 \pm 0.1$ and 0.45 ± 0.1 on the square lattice and simple cubic lattice respectively. The exponent Δ appears to be a universal quantity for a given dimension. That is to say, it appears to be independent of the bridge length b. The leading term A decreases monotonically with increasing bridge length, as would be expected intuitively. The sub-dominant amplitude B also appears to decrease with increasing bridge length, and displays a trend to a distinct limit according as N is even or odd for $b=2$. As we see from the $b=1$ data, these estimates approach a common limit for N sufficiently large. Presumably this will also occur for the $b=2$ data, but our series are too short to display this behaviour. All the numerical values are summarized in table 3.

Barat *et al* have argued that a further correction term is necessary in equation (1) if the true asymptotic behaviour is to be seen. They have assumed the form

$$R_N \sim A + N^{-\Delta}(B + C/N). \tag{3}$$

We argue that this is most unlikely to be correct. The dominant term A in (1) is not

Table 3. A, B and Δ from series analysis of the shortest path data of SAWs on square and simple cubic lattices.

	A				B				Δ			
	$b=1$		$b=2$		$b=1$		$b=2$		$b=1$		$b=2$	
N	$d=2$	$d=3$	$d=2$	$d=3$	$d=2$	$d=3$	$d=2$	$d=3$	$d=2$	$d=3$	$d=2$	$d=3$
7	0.62187	0.52767	0.27247	0.19395	0.41230	0.58867	0.84736	0.71290	0.53135	0.43340	0.88604	0.75008
8	0.62641	0.57220	0.25194	0.16401	0.48085	0.64775	0.32031	0.50022	0.58539	0.56598	0.55665	0.51465
9	0.67388	0.49036	0.27546	0.20379	0.43792	0.61010	0.85591	0.72704	0.78747	0.38117	0.90149	0.79163
10	0.66555	0.52755	0.28132	0.13727	0.52682	0.64811	0.34797	0.50497	0.78391	0.46918	0.76248	0.44954
11	0.67059	0.48465	0.27259	0.20291	0.42816	0.61284	0.84052	0.72420	0.75830	0.37347	0.88229	0.78673
12	0.67166	0.51872	0.28468	0.14951	0.55480	0.64791	0.36127	0.50557	0.83815	0.45197	0.80367	0.48075
13	0.67208	0.48648	0.27382	0.19509	0.43473	0.61224	0.85029	0.69040	0.77371	0.37611	0.89219	0.73811
14	0.67573	0.51670	0.28523		0.58888	0.64746	0.36487		0.88655	0.44783	0.81226	
15	0.67243		0.27569		0.43696		0.87191		0.77800		0.91052	
16	0.67607		0.28345		0.59311		0.35058		0.89154		0.78165	
17	0.67374		0.27755		0.44817		0.90208		0.79655		0.93248	
18	0.67624		0.28250		0.59582		0.34213		0.89442		0.76437	
19	0.67407		0.27873		0.45182		0.92783		0.80190		0.94897	
20	0.67639		0.28188		0.59861		0.33605		0.89714		0.75251	
21	0.67427		0.27954		0.45459		0.95037		0.80561		0.96200	
22	0.67639		0.28133		0.59868				0.89720		0.74153	
23	0.67448				0.45798				0.80985			
24	0.67632				0.59693				0.89568			
∞	0.675 ± 0.005	0.50 ± 0.05	0.281 ± 0.004	0.18 ± 0.05	0.55 ± 0.05	0.63 ± 0.04	0.3 (n even) 1.0 (n odd)	0.60 ± 01	0.86 ± 0.10	0.41 ± 0.05	0.86 ± 0.20	0.6 ± 0.2

going to be a pure constant, but at best an analytic function. In that case, the next correction term will be $O(1/N)$, not $O(1/N^{1+\Delta})$ as assumed. If A (or B) is not analytic, other correction terms will appear.

These considerations then suggest that the simple, analytic assumption, $\Delta = 1$ is appropriate for the square lattice data. For the simple cubic lattice, the corresponding analysis, shown in table 3, displays quite different behaviour, implying that Δ is around 0.5.

For the square lattice data, we next extrapolated the sequence $\{R_N\}$ by Neville-Aitken extrapolation to the odd and even sub-sequence independently, and also analysed the data by fitting successive alternative coefficients R_K, R_{K-2}, R_{K-4} and R_{K-6} to the form

$$R_N \sim A + BN^{-1} + CN^{-\Lambda} \tag{4}$$

where we expect $\Lambda > 1$. Neville-Aitken extrapolation (not shown) allows us to estimate $A = 0.677 \pm 0.004$ for $b = 1$, $A = 0.445 \pm 0.005$ for $b = \sqrt{2}$, $A = 0.283 \pm 0.005$ for $b = 2$. Attempts to estimate Λ from (4) were unsuccessful. However, in the light of the expected behaviour of ordinary SAWs in which the leading correction is analytic and the next correction has exponent 1.5 [6], it is plausible that the corresponding exponent $\Lambda = 1.5$ also. If we make this assumption, successive triples of alternate coefficients R_K, R_{K-2} and R_{K-4} yield estimates of A, B and C from (4).

Compared with table 3, the estimates of A and B so obtained were better converged and do not show the odd-even dependence of table 3 estimates—though estimates of C still display this feature. Extrapolating these results, we found for $b = 1$ that $A = 0.677 \pm 0.003$, $B = 1.0 \pm 0.1$, $C \simeq 1$. The estimate of the leading amplitude A is in agreement with our earlier analysis above, and the fit is altogether more satisfactory.

For the simple cubic data, Neville-Aitken extrapolation is inappropriate given the non-integral estimate of Δ. However, as $\Delta \simeq \frac{1}{2}$, and again we expect analytic corrections to (1), we fitted successive alternative triples to

$$R_N \sim A + BN^{-1/2} + CN^{-1}. \tag{5}$$

Extrapolation of these results for $b = 1$ gave $A = 0.52 \pm 0.01$, $B = 0.8 \pm 0.1$, $C = -0.4 \pm 0.2$. Again, we find the fit to (5) altogether more satisfactory than the fit to (4) shown in table 3.

In order to analyse the Monte Carlo data, the generation of which is discussed subsequently, we used a method derived by Yeramian and Claverie [7] and Claverie *et al* [8] based on Mellin-Padé transformations. We first note that as the shortest path length between two sites of a SAW configuration cannot exceed the chain length between them, we can write quite generally

$$R_N \sim \sum_{i=1}^{\infty} D_i N^{-\mu_i} \tag{6}$$

with $D_1 = A$, $D_2 = B$, $\mu_1 = 0$, $\mu_2 = \Delta$, $\mu_i \geqslant 0$ and $\mu_i < \mu_{i+1}$. After taking a Mellin transform [9, 10], equation (6) becomes:

$$\bar{R}(p) \equiv \int_1^{\infty} N^{p-1} R_N \, \mathrm{d}N \sim -\sum_{i=1}^{\infty} \frac{D_i}{p - \mu_i} \qquad p < 0. \tag{7}$$

Expanding $\bar{R}(p)$ around $p_0 < 0$, we have

$$\bar{R}(p) = \sum_{n=0}^{\infty} E_n(p_0)(p - p_0)^n \tag{8}$$

with

$$E_n(p_0) = \frac{1}{n!}\int_1^\infty (\ln N)^n N^{p_0-1} R_N \, dN. \tag{9}$$

From the estimates of R_N, the integral (9) is performed numerically to give estimates of $E_n(p_0)$. Given $E_n(p_0)$, we can get an expression for $\tilde{R}(p)$ from (8), and from Padé approximants [11] to the series (8) so derived, we estimate μ_i and D_i from (7).

In the numerical calculation, however, we can only get the values of R_N at finite integer values of N. The integrations in (9) cannot therefore be carried out exactly. Nevertheless, as R_N becomes flat for large N and the scaling behaviour is determined by the large N limit, the error involved in taking the discrete values for R_N is negligible for $N \to \infty$. The small N error can be reduced by using standard numerical integration methods such as Simpson's rule [12].

The leading contribution to the integration in (9) is the term in R_N with the smallest exponent. Hence, $E_n(p_0)$ can be approximated by

$$E_n(p_0) \simeq \frac{1}{n!}\int_1^{N_0} (\ln N)^n N^{p_0-1} R_N \, dN + \frac{1}{n!}\int_{N_0}^\infty (\ln N)^n N^{p_0-1} A^+ \, dN. \tag{10}$$

Here $A^+ \geqslant A$ is a constant.

The Monte Carlo data were generated using the constant fugacity Monte Carlo enumeration method [13]. For $b = 1$, we generated 25 000 000 SAW configurations of 300 steps on the 600×600 square lattice. The shortest path is calculated with the same site labelling method as that for the series expansion. To get better statistics, we labelled the middle site, i.e., the 150th, site as 0. Take $N_0 = 150$ and $A^+ = (A + R_{150})/2$, where $A = 0.677$ from the series result, and the coefficients $E_n(p_0)$ are calculated for $p_0 = [-6, -3]$. The Padé approximation estimates of E_n calculated as above were consistent with the series expansion predictions, although with larger error bars. The Mellin–Padé analysis to the shortest path of the SAWs with $b = \sqrt{2}$ and 2 on the square lattice gave similar results. An alternative, simpler analysis in which we fitted the Monte Carlo data to (1) was inconclusive.

3. Discussion

In this paper, we have studied the correction to scaling of the shortest path on the 'SAWs with bridges' model by extensive numerical simulation. The results we get in the present study are consistent using different methods of numerical analysis, but are not consistent with earlier studies. We argue that the inconsistency results from inappropriate methods used in earlier works.

We find indeed that, in two dimensions, the leading correction exponent is likely to be analytic, while in three dimensions it is near $\frac{1}{2}$. This is similar to the correction-to-scaling behaviour of ordinary self-avoiding walks.

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