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COMMENT

Shortest path of SAWs with bridges: series results

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Abstract. Recent Monte Carlo simulation results of Yang and Chakrabarti suggest the shortest path S_N of an N-stepped self-avoiding walk (SAW), with finite range interaction of bridges, has a finite size scaling behaviour $S_N/N \simeq A + N^{-\Delta}(B + C/N)$, where the exponent Δ is superuniversal; $\Delta \simeq 0.19$ for all dimensions d studied ($2 \leqslant d \leqslant 5$). We report here the small-N series enumeration results for S_N for SAWs with nearest-neighbour bridges on square (up to $N = 18$), triangular (up to $N = 11$) and simple cubic (up to $N = 12$) lattices. The estimated values of Δ for different lattices ($\simeq 0.22 \pm 0.01$ for $d = 2$ and $\simeq 0.26 \pm 0.01$ for $d = 3$) have been compared with the above Monte Carlo estimate and the indication of superuniversal behaviour of Δ has been discussed.

The multifractal properties of self-avoiding walks (SAWs) with (say nearest-neighbour) bridges networks [1] are of current interest. For example, the resistance $R_N \sim N^{\delta}$ of a SAW chain of length N (bridge bonds having identical resistance to the chain bonds) with δ ($\leqslant 1$) as the resistance exponent [2-4], the shortest path length $S_N \sim N^{\varepsilon}$ where ε ($\leqslant 1$) is the shortest path exponent [1, 4-6] and the spectral dimension d_s ($\geqslant 1$) [1, 3, 4, 7, 8] of such networks have been studied extensively. On careful analysis [1] the results of all these studies (for $d = 2$ and 3) indicate the SAW with bridges network to be dominantly linear in structure ($\delta = \varepsilon = d_s = 1$). In fact, since the diffusion on the network is related to its conductivity, δ is related to d_s by a scaling relation [4] $d_s = 2/(1+\delta)$. Also one expects on general grounds [6], $\delta \leqslant \varepsilon$. Such networks are expected to become linear above the upper critical dimension $d = 4$ for SAWs, and are obviously linear in $d = 1$. All the above results [1-8] for $2 \leqslant d < 4$, derived independently, become mutually consistent: $\delta = \varepsilon = d_s = 1$ for all d. However, significant finite size scaling corrections to this linear scaling behaviour are expected due to the local blobs coming from the multiply connected structures formed due to the local bridges. The above quantities, say the average shortest path length S_N, are expected to have scaling form [1],

$$S_N/N \simeq A + N^{-\Delta}(B + C/N) \tag{1}$$

where A, B and C are constants dependent on the lattices (and the bridge length or interaction range etc). The parameter A denotes the fraction of SAW steps which are not connected to the other parts of the SAW by bridges (the exponent ε for S_N, discussed before, is taken to be unity). The recent Monte Carlo simulation results for the shortest

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path of SAWs (with $N \sim 150$ for $d = 2$ to $N \sim 25$ for $d = 5$) indicated [1] the exponent Δ to be superuniversal; $\Delta \simeq 0.19$ for all the dimensions studied ($2 \leqslant d \leqslant 5$).

Here we intend to compare and check the observation using series enumeration results for shortest paths of SAWs with nearest-neighbour bridges. We have obtained the series results for S_N on square, triangular and simple cubic lattices for step sizes N up to 18, 11 and 12 respectively. We have found A, B and C from least-squares fits to equation (1) and then obtained the extrapolated values of Δ in $d = 2$ and 3. These values of Δ have been compared with the Monte Carlo estimate.

We use the Martin algorithm [9] for enumerating the SAW configurations. The shortest path S_N (through nearest bridges) for each SAW configurations can be found out using the labelling algorithm [1, 4]. The linear part (A_N) of each SAW configuration, the part of the network for which there is no multiple connection through the bridges, has also been independently determined. The results for the total number (C_N) of SAW configurations of N steps, total shortest path length ($C_N S_N$) and the total linear part ($C_N A_N N$) for SAWs on square (up to $N = 18$), triangular (up to $N = 11$) and simple cubic (up to $N = 12$) lattices are given in table 1. The calculations took about 60 CPU hours on a Horizon III and 15 CPU hours on a ND-500 computer.

In figure 1 we have presented the value of A_N (obtained from series enumeration of the linear part from table 1) as a function of $1/N$, for different lattices. In order to evaluate Δ, the asymptotic values of the constants A, B and C are needed. From the analysis of these linear part data, A values can be estimated. We use Padé approximants for A_N (as ratios of polynomials in $1/N$ of order m and n, $m < n$, with coefficients to be determined from chosen values of m and n). This method is quite stable and the estimated values of A are 0.55 ± 0.01, 0.326 ± 0.001 and 0.46 ± 0.01 for square, triangular and simple cubic lattices respectively. An independent least-squares fit of the shortest path data to equation (1), gives the values of A, B and C which are presented in table 2 (allowed standard deviation is of the order of 10^{-6}). The value of A for the triangular lattice obtained from the above two independent methods are found to be in good agreement, whereas the agreements are not apparent for square and cubic lattice estimates. This discrepancy can be understood from figure 1. This figure reveals that for square and simple cubic lattices the size dependence of A_N fluctuations are quite strong from the small step sizes considered (this fluctuation is rather small for the triangular lattice). It may be noted, however, that the least-squares fit to the Monte Carlo estimate of S_N in [1] gave A, B and C values, which, in most cases, are within the error limits of our least-squares fit estimate from series enumeration results. This suggests that the values of A, B and C obtained by a least-squares fit of the S_N data, even for the small step sizes considered here, are quite reliable. In figure 2, we have plotted Δ_N as a function of $1/N$ using our least-squares fit values of A, B and C, given in table 2. They appear to extrapolate to the values $\Delta \simeq 0.23$ for square, $\Delta \simeq 0.20$ for triangular and $\Delta \simeq 0.26$ for simple cubic lattices. Although these values of Δ (and its dimensional variation observed here) do not compare very well with the previous Monte Carlo estimate [1] of a superuniversal (d-independent) value of Δ ($\simeq 0.19$), the extrapolated estimates from such small series analysis are not very reliable either.

It should be mentioned that putting $C = 0$ in equation (1), we had also estimated Δ_N using a second method: solving numerically for $f(N, \Delta_N) = 0$, where

$$f(N, \Delta_N) = [(S_N/N) - (S_{N-2}/(N-2))]/[(S_{N-2}/(N-2)) - (S_{N-4}/(N-4))] - [N^{-\Delta} - (N-2)^{-\Delta}]/[(N-2)^{-\Delta} - (N-4)^{-\Delta}].$$

Table 1. C_N, S_N and A_N for SAWs with nearest-neighbour bridges on square, triangular and simple cubic lattices.

Lattice type	No of steps N	No of SAW configurations C_N	Total shortest path length S_NC_N	Total linear path length A_NNC_N
Square	1	4	4	4
	2	12	24	24
	3	36	92	84
	4	100	336	304
	5	284	113 2	996
	6	780	372 0	325 6
	7	217 2	116 84	100 84
	8	591 6	363 84	312 96
	9	162 68	110 028	938 92
	10	441 00	331 720	282 360
	11	120 292	979 276	829 380
	12	324 932	288 846 4	244 142 4
	13	881 500	838 641 2	706 383 6
	14	237 444 4	243 491 60	204 760 24
	15	641 659 6	698 355 48	585 759 72
	16	172 453 32	200 362 176	167 835 408
	17	464 666 76	569 268 356	475 906 532
	18	124 658 732	161 817 2568	135 129 3944
Triangular	1	6	6	6
	2	30	48	36
	3	138	306	210
	4	618	174 0	115 2
	5	273 0	929 4	599 4
	6	119 46	476 40	302 04
	7	518 82	237 102	148 362
	8	224 130	115 419 6	714 912
	9	964 134	552 262 2	339 300 6
	10	413 316 6	260 613 84	159 048 84
	11	176 689 38	121 596 186	737 941 38
Simple cubic	1	6	6	6
	2	30	60	60
	3	150	402	378
	4	726	252 0	232 8
	5	353 4	145 02	130 38
	6	169 26	819 72	729 00
	7	813 90	444 930	390 306
	8	387 966	239 563 2	208 603 2
	9	185 388 6	125 872 14	108 680 70
	10	880 987 8	658 601 88	565 563 00
	11	419 341 50	339 003 810	289 407 114
	12	198 842 742	174 062 2920	147 974 8968

Such a method gives $\Delta \simeq 0.8$–0.9 for $d=2$ and $\Delta \simeq 0.5$ for the simple cubic lattices†. However, the error in such a method is obvious. As mentioned previously, and shown

† Such large values of Δ ($\simeq 0.8$ for $d=2$) have also been obtained [10] for similar small series results for SAWs on the square lattice [6] by employing a similar method (treating A_N independent of N) (from series for N up to 22 in the square lattice).

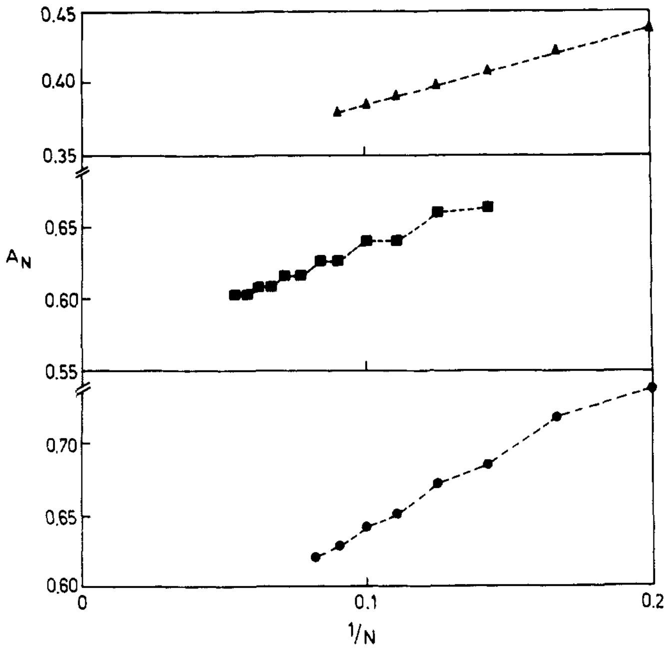

Figure 1. A_N against $1/N$, from table 1, for various lattices (■: square; ▲: triangular; ●: simple cubic).

Table 2. Values of A, B, C and Δ from least-squares fit to (1) of the S_N data from table 1.

Lattice	A	B	C	Δ
Square	0.498 ± 0.001	0.466 ± 0.001	-0.04 ± 0.1	0.257 ± 0.001
Triangular	0.326 ± 0.001	0.516 ± 0.001	-0.04 ± 0.01	0.227 ± 0.001
Simple cubic	0.391 ± 0.01	0.628 ± 0.03	0.21 ± 0.1	0.26 ± 0.1

in figure 1, the variation in A_N for such small step sizes is quite large and the error in taking it as a constant, in this method, forces the entire change in S_N (contributed by both changes in A_N, which for $N \simeq 18$ accounts for almost the entire change in S_N, and in $N^{-\Delta}$ terms in (1) with $c = 0$) to be determined by Δ alone, giving naturally large value of Δ.

We have fitted here to equation (1) the small series data for the shortest path length S_N of SAWs with nearest-neighbour bridges. The least-squares fit gives the fitting values of the parameters (A, B, C and Δ) comparable to those obtained fitting the large-N Monte Carlo data [1] for S_N. We also obtained independently the fraction of steps A_N which are not connected to other parts of the SAW by bridges. These also gave comparable estimates of A ($=A_N$, $N \to \infty$). The sequences of Δ_N are obtained from the least-squares fit (of S_N to equation (1)) parameter values. The extrapolated values of Δ ($\simeq 0.22 \pm 0.02$ in $d = 2$ and $\simeq 0.26 \pm 0.01$ in $d = 3$) compare well with the Monte Carlo indication [1] of superuniversality of the exponent Δ ($\simeq 0.19$). It is found that for the triangular lattice series, even this small size gives quite a smooth variation in Δ_N and extrapolates to $\Delta \simeq 0.20$, which is close to the Monte Carlo estimate [1]. It

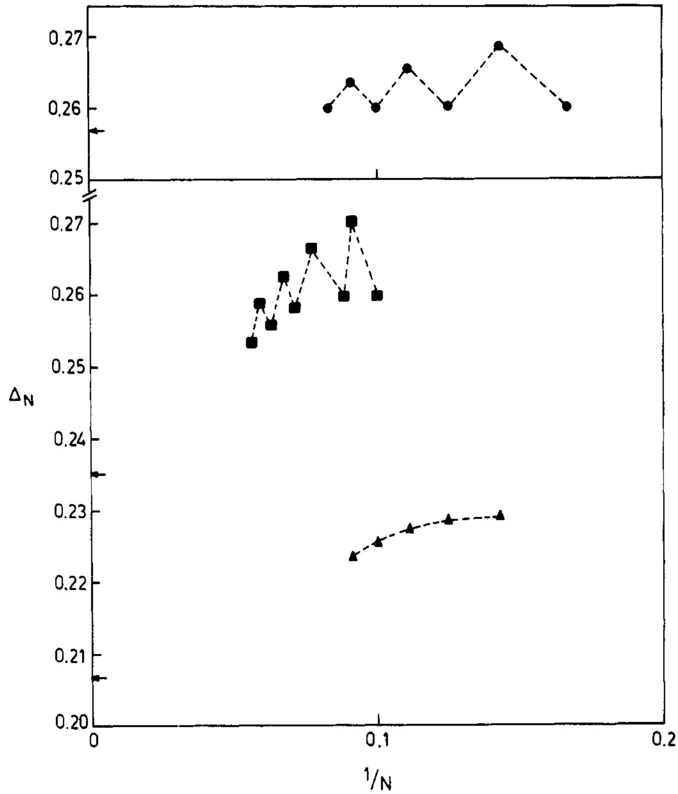

Figure 2. Δ_N obtained from (1), using a least-squares fit estimate of A, B, C and Δ. The extrapolated estimates of Δ are indicated by the horizontal arrows (■: square; ▲: triangular; ●: simple cubic).

thus indicates that because of even–odd fluctuations, the square and simple cubic lattice data are not yet sufficient and slightly larger series data would probably give the (superuniversal) Δ value close to the Monte Carlo estimate.

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