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Non-universal behaviour of self-attracting walks

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Abstract. A recently proposed model for self-attracting walks is studied using exact enumeration techniques. The probability of a step is proportional to $\exp(-nu)$, where n = 1 for sites already visited by the walker and n = 0 for the others, with u < 0. Series for the mean-square displacement $\langle R_N^2 \rangle \sim N^{2\nu}$ and the mean number of visited sites $\langle S_N \rangle \sim N^3$ of N-step walks are calculated in one to four dimensions. In all dimensions anomalous diffusion is observed, and exponents ν and s vary continuously with the strength parameter u. The results are compared with simulations and with previous results for static and dynamic models of generalized random walks in one dimension. The behaviour in two and three dimensions may describe anomalous diffusion in real systems.

1. Introduction

Random walks (RW) and interacting random walks (with memory) model many physical processes. RW are applied as a model for transport phenomena [1,2] and the more intensively studied interacting walk, the self-avoiding walk (SAW), describes the properties of polymers in solution [3,4]. The mean-square end-to-end distance of N-step walks behaves asymptotically as

$$\langle R_N^2 \rangle \sim N^{2\nu} \,. \tag{1}$$

For RW, $\nu = \frac{1}{2}$ in all dimensions, and for SAW $\nu > \frac{1}{2}$ for up to three dimensions. When $\nu < \frac{1}{2}$ the walk is antipersistent and is said to display anomalous diffusion. This is a characteristic of RW in fractal systems [2].

Other interacting random walks of physical interest have also been studied, such as the true self-avoiding walk (TSAW) [5,6], the Domb-Joyce model [7] and an interacting walk of Stanley *et al* [8,9]. A comparative study of these models in one dimension [10] has shown that the particular form of correlation between steps is fundamental to the critical behaviour. Some of the important mechanisms are the range of the interaction, the presence of cumulative memory effects and global or local normalization conditions [10].

Unifying models of static and dynamic random walks have been proposed, including the previous models as limiting cases. Duxbury and de Queiroz [11] studied a generalized random walk in which each configuration with N steps has weight

$$W = \exp\left(-g\sum_{i=1}^{S} (n_i)^{\alpha}\right)$$
⁽²⁾

where the sum spans all S visited sites and n_i is the number of times site *i* is visited. The parameter g determines the strength of the correlation between steps and the exponent α

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varies from 0 to 2 (RW corresponds to $\alpha = 1$). The asymptotic behaviour in one dimension depends on the exponent α . The interacting walk of Stanley *et al* [8] corresponds to $\alpha = 0$ and, in the attracting case (all g < 0), displays anomalous diffusion with $\nu = \frac{1}{3}$ [9].

The above static model has a corresponding dynamic model proposed by Öttinger [12]. In this generalized model the probability p_i for moving to a site *i* is proportional to

$$W_i = \exp(-gn_i^{\alpha}). \tag{3}$$

The one-dimensional version was studied for $0 < \alpha \leq 2$ and g > 0, and it was shown that v depends on α but not on g [12].

Recently, Sapozhnikov [13] studied a generalized walk in which the probability for the walker to jump to a site is proportional to

$$p = \exp(-nu) \tag{4}$$

where n = 1 for the sites visited by the particle at least once and n = 0 for the others. This model is the limit $\alpha \to 0$ of Öttinger's model. The case u < 0 was called a self-attracting walk (SATW). Computer simulations gave $\nu < \frac{1}{2}$ for u = -1 and u = -2 in dimension D = 2, and it was proposed that $\nu = \frac{1}{2}$ in D = 1 and $\frac{1}{4} < \nu < \frac{1}{3}$ in D = 3 [13].

The possibility of anomalous diffusion in two and three dimensions is interesting because there are experiments which show this property [13, 14] and previous theoretical papers were limited to one-dimensional systems.

The purpose of this paper is to study SATW by exact enumeration of short walks (series expansions), obtaining estimates of the exponent v and the exponent s defined by

$$\langle S_N \rangle \sim N^s$$
 (5)

where $\langle S_N \rangle$ is the mean number of sites visited by N-step walks. In section 2 we present the enumeration techniques, an example of the calculation of the probability of two walks and the techniques used for series analysis. In section 3 we present accurate results in D = 1 for several values of the parameter u, obtained from series up to N = 30. In section 4 we show the results for D = 2, obtained from series for the square and the triangular lattice. The comparison of the estimates of the exponent v for these two lattices is convenient to test the extrapolation procedure. In section 5 we show the results for D = 3 and 4, and the paper concludes in section 6 with a summary and discussion.

2. Series generation and analysis

In order to calculate $\langle R_N^2 \rangle$ (equation (1)) and $\langle S_N \rangle$ (equation (5)) we have to consider all walks with N steps (z^N walks, where z is the lattice coordination number), and the probability P_{α} of each walk α . Then

$$\langle R_N^2 \rangle = \sum_{\alpha=1}^{z^N} P_\alpha R_\alpha^2 \tag{6}$$

and

$$\langle S_N \rangle = \sum_{\alpha=1}^{z^N} P_\alpha S_\alpha \tag{7}$$



Figure 1. (a) Walk with six steps initiated at site O and ending at site A. (b) Walk whose seventh step is from A to B (site B was not visited yet). (c) Walk whose seventh step is from A to C (site C was already visited). The walk in (c) has probability $e^{-\mu}$ times greater than the probability of the walk in (b). E and D are the other sites available for the seventh step.

where R_{α}^2 and S_{α} are the square end-to-end distance and the number of visited sites of walk α , respectively. The probability P_{α} is given by

$$P_{\alpha} = \prod_{i=1}^{N} P_{i,\alpha} \tag{8}$$

where $P_{i,\alpha}$ is the probability of the *i*th step in walk α , obtained using (4). This probability is given by

$$P_{i,\alpha} = \frac{\exp(-n_{s_i}u)}{\sum_{i=1}^{z} \exp(-n_{j}u)}.$$
(9)

The sum in (9) is over the nearest neighbours of the *i*th site of walk α (the end of the walk up to the (i - 1)th step); s_i is the site to where the walker jumps in the *i*th step of walk α ; $n_i = 1$ or 0 if the neighbouring site *j* has already been visited or not, respectively.

As an example, consider the walks in figure 1. Let P be the probability of the walk up to six steps (from O to A, figure 1(a)). As site A has two neighbours previously visited (C and D), the probability of the walk in figure 1(b) is $P(2 + 2e^{-u})^{-1}$, and the probability of the walk in figure 1(c) is $Pe^{-u}(2 + 2e^{-u})^{-1}$. The former probability also applies to a walk which jumps from A to E and the latter to a walk which jumps from A to D.

As we will study the case u < 0, it is more probable that the walker jumps to the previously visited sites C and D. Both steps have the same probability because the attractive effect is not cumulative, i.e. it does not depend on the number of visits to a site. This is a characteristic of the model of Stanley *et al* [8,9], with the difference of the local normalization condition of SATW, as shown in the example above.

The estimates of the exponents v (1) and s (5) are obtained through the ratio method [15]. As the series for SATW are very regular for small values of u, this technique gives accurate results. More sophisticated methods, like Padé approximants, on the other hand, do not work well for those series [16].

As the series frequently present oscillations, we treat even and odd N separately, defining the ratios of successive terms

$$p_N = \frac{\langle R_N^2 \rangle}{\langle R_{N-2}^2 \rangle} \tag{10a}$$

and

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$$\mu_N = \frac{\langle S_N \rangle}{\langle S_{N-2} \rangle} \,.$$

(10b)

Initial estimates of v and s are obtained from

$$\nu_N = \frac{1}{4}N(\rho_N - 1)$$
 (11a)

and

$$s_N = \frac{1}{2}N(\mu_N - 1) \tag{11b}$$

so that $\nu_N \rightarrow \nu$ and $s_N \rightarrow s$ for $N \rightarrow \infty$. Corrections to scaling in (1) and corrections to the approximation $\rho_N \approx 1 + 4\nu/N$ (equations (1) and (10*a*)) are responsible for the differences between ν_N and ν . Similar corrections appear when $s_N \rightarrow s$. The sequences $\{\nu_N\}$ and $\{s_N\}$ are analysed by constructing Neville tables, where they are considered as functions of 1/N [15]. The first column of these tables gives the intercepts with the 1/N = 0 axis of straight lines passing through each pair of successive points of the plot ν_N (or s_N) versus 1/N; these estimates are

$$\nu_N^{(1)} = \frac{1}{2} (N\nu_N - (N-2)\nu_{N-2}) \tag{12a}$$

and

$$s_N^{(1)} = \frac{1}{2}(Ns_N - (N-2)s_{N-2})$$
(12b)

where even and odd N are considered separately, as before.

 $\nu_N^{(1)}$ and $s_N^{(1)}$ represent the first step to reduce the corrections cited above. Their convergence can be analysed with the same techniques. Sequences $\{\nu_N^{(2)}\}$ and $\{s_N^{(2)}\}$ are obtained by extrapolating $\{\nu_N^{(1)}\}$ and $\{s_N^{(1)}\}$ with the transformations applied to $\{\nu_N\}$ and $\{s_N\}$ in (12*a*) and (12*b*). The application of these extrapolations procedures is important until the convergence is well stablished, i.e. when successive extrapolations provide similar estimates of the exponents. In general, the convergence properties of $\nu_N^{(1)}$ and $s_N^{(1)}$ will give accurate estimates of ν and s.

3. SATW in one dimension

We calculated $\langle R_N^2 \rangle$ and $\langle S_N \rangle$ up to N = 30 for several values of the parameter u, ranging from -0.2 to -3.0. In table 1 we present the results for u = -1.0, the only value for which series up to order 35 were calculated.

In figure 2 we plot $v_N \times 1/N$ (equation (11*a*)) for u = -0.2 and -1.0 and in figure 3 we plot $v_N^{(1)} \times 1/N$ (equation (12*a*)) for the same values of *u*. Note that for u = -1.0 the plots in figures 2 and 3 seem to give different estimates of *v*. However, the sequence $\{v_N^{(1)}\}$ can be extrapolated according to the procedure described in section 2 and we obtain the sequence $\{v_N^{(2)}\}$, shown in figure 4 also as function of 1/N. The last values of $v_N^{(2)}$ confirm the trend to $v \approx 0.47$ in figure 3.

The convergence of the plots in figure 3 indicates that $\nu < \frac{1}{2}$ in both cases, proving that even for small relative probabilities ($e^{0.2} \approx 1.22$) anomalous diffusion is found. For greater values of |u|, the even-odd oscillations of those plots are greater, then it is possible to estimate ν accurately (with an error less than 10%) only up to |u| = 2.0.

In table 2 we show the final estimates of ν , obtained with the same procedure described above for u = -1.0. It seems that ν decreases continuously when u decreases, increasing the attraction effect. This result is different of the universal behaviour ($\nu = \frac{1}{3}$) obtained



Figure 2. Plot of $v_N \times 1/N$ (equation (11*a*)) for u = -0.2 (\Box) and u = -1.0 (O) in one dimension.

Table 1. $\langle R_N^2 \rangle$ and $\langle S_N \rangle$ for u = -1.0 in one dimension.

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N	$\langle R_N^2 \rangle$	$\langle S_N \rangle$
2	1.075 765 685 479	2.268 941 421 370
3	1.578 635 905 028	2.537 882 842 739
4	1.702 418 296 093	2.753 947 171 325
5	2.085 357 524 949	2.970 011 499 911
6	2.249 567 330 012	3.150 705 423 395
7	2.565 809 081 498_	3.333 042 270 474
8	2.751 981 334 734	3.489 941 634 627
9	3.029 670 676 011	3.649 228 764 791
10	3.225 938 276 476	3.789 466 303 981
11	3.480 440 840 353	3.932 159 557 364
12	3.680 517 339 792	4.060 157 797 637
13	3.920 371 229 655	4.190 363 955 481
14	4.121 184 199 112	4.308 953 615 730
15	4.351 226 221 383	4.429 400 916 947
16	4.551 378 015 262	4.540 470 653 181
17	4.774 423 491 206	4.653 047 210 016
18	4.973 348 986 452	4.757 914 090 864
19	5.191 099 651 610	4.863 977 524 063
20	5.388 630 372 734	4.963 599 965 956
21	5.602 166 230 659	5.064 160 631 486
22	5.798 311 407 887	5.159 263 199 186
23	6.008 357 992 179	5.255 095 810 021
24	6.203 197 705 039	5.346 244 336 342
25	6.410 272 115 881	5.437 958 122 307
26	6.603 907 217 057 .	5.525 606 389 051
27	6.808 398 714 049	5.613 690 670 442
28	7.000 928 932 422	5.698 210 465 906
29	7.203 144 151 757	5.783 065 250 873
30	7.394 659 781 711	5.864 766 454 171
31	7.594 848 781 737	5.946 723 634 044
32	7.785 428 599 646	6.025 868 116 449
33	7.983 800 392 678	6.105 206 565 032
34	8.173 512 205 359	6.182 018 294 338
35	8.370 244 545 295	6.258 974 993 396



Figure 3. Plot of $v_N^{(1)} \times 1/N$ (equation (12a)) for u = -0.2 (\Box) and u = -1.0 (O) in one dimension.



Figure 4. Plot of $v_N^{(2)} \times 1/N$ (see text) for u = -1.0 in one dimension.

Table 2. Estimates of v and s in one dimension, for several values of the strength parameter u.

u	ν	5
-0.2	0.490 ± 0.005	0.496 ± 0.004
-0.5	0.48 ± 0.01	0.488 ± 0.006
-1.0	0.465 ± 0.015	0.475 ± 0.010
-1.5	0.44 ± 0.02	0.465 ± 0.015
2.0	0.42 ± 0.03	0.445 ± 0.020

for the corresponding static model [9]. In the dynamic case, it is clear the non-universal behaviour and, at least for $|u| \leq 2.0$, the attraction effect is weaker (all $\nu > \frac{1}{3}$ in table 2). As we cannot obtain accurate estimates for |u| > 2.0, it is not possible to decide whether ν crosses the value $\frac{1}{3}$ or converges to it for $u \to -\infty$. We will return to this point in section 6.

In figure 5 we plot $s_N^{(1)} \times 1/N$ (equation (12b)) for u = -0.5 and u = -1.5. We



Figure 5. Plot of $s_N^{(1)} \times 1/N$ (equation (12b)) for u = -0.5 (\Box) and u = -1.5 (\odot) in one dimension.

also see that $s < \frac{1}{2}$ even for small values of u ($s = \frac{1}{2}$ for RW [1]). On the other hand, the even-odd oscillations of $s_N^{(1)}$ do not increase quickly with |u| as in the plots of $v_N^{(1)}$, so that we are able to obtain estimates of s up to u = -3.0. The final estimates of s for the values of u in which we found estimates of v are also shown in table 2.

It is expected that v = s in one dimension [9, 10]. Our results for SATW do not discard this possibility (see table 2) but all the centres of the error bars indicate v < s. It means that the number of visited sites grows faster than the end-to-end distance. This is not completely surprising because slightly different behaviours of $\langle R_N^2 \rangle$ and $\langle S_N \rangle$ were already noted, for instance in the one-dimensional Domb-Joyce model in the attractive regime [10]: although v = s = 0, $\langle S_N \rangle$ saturates and $\langle R_N^2 \rangle$ collapses.

Our results disagree with the proposal of Sapozhnikov that $v = \frac{1}{2}$ for all u in one dimension [13]. His arguments are based on the hypothesis that the walker can be localized at any visited site with equal probability when $N \rightarrow \infty$. However, this is a property of RW and not necessarily of SATW. In fact, our numerical results show that these arguments fail for SATW.

4. SATW in two dimensions

We calculated $\langle R_N^2 \rangle$ and $\langle S_N \rangle$ up to N = 18 for the same values of u of the one-dimensional case in the square lattice. We performed the same calculations in the triangular lattice up to N = 14.

In table 3 we show the results for u = -1.0. In figure 6 we plot $v_N \times 1/N$ (equation (11*a*)) for u = -0.5 and -1.0 in both lattices. For the greatest odd values of N the results are almost identical (the even-odd oscillations are characteristic of loose-packed lattices, such as the square lattice). It seems that the estimates converge to the same v, which is an expected universal behaviour.

In table 4 we show the final estimates of v, using the square lattice data and the same extapolation procedures applied to the one-dimensional case. It is possible to obtain accurate estimates only up to u = -2.5.



Figure 6. Plot of $v_N \times 1/N$ (equation (11a)) for u = -0.5 and u = -1.0 in the square (\Box) and the triangular (Δ) lattices. The empty polygons correspond to u = -0.5 and the full ones to u = -1.0.

Table 3. $\langle R_N^2 \rangle$ and $\langle S_N \rangle$ for u = -1.0 in the square and the triangular lattices.

N	$\langle R_N^2 \rangle_{sq}$	$\langle S_N \rangle_{sq}$	$\langle R_N^2 \rangle_{tr}$	$\langle S_N \rangle_{tr}$
2	1.399 021 636 216	2.524 633 113 581	1.554750171955	2.647 812 571 648
3	1.978 630 769 301	3.049 266 227 162	2.124 761 322 697	3.237 599 416 485
4	2.348 917 622 092	3.494 492 334 085	2.606 175 078 874	3.760 838 777 819
5	2.824 927 196 295	3.938 454 572 075	3.077 419 603 973	4.253 189 963 116
6	3.180 776 420 424	4.336 691 109 141	3.515 031 981 260	4,714 312 265 268
7	3.602 504 197 147	4.735 080 374 590	3.940 600 196 302	5.155745856066
8	3.945 851 968 515	5.102 548 790 700	4.348 573 891 303	5.578 517 785 186
9	4.334 019 253 009	5.470 783 830 243	4.746 447 661 788	5.987 377 949 360
10	4.666 304 961 349	5.816 252 479 833	5.133 074 800 632	6.383 431 559 116
11	5.031 448 866 637	6.162 668 024 753	5.511 571 457 832	6.769 006 177 735
12	5.354 122 412 350	6.491 384 971 853	5.881 958 059 743	7.145 018 594 754
13	5.702 288 193 019	6.821 066 307 471	6.245 741 349 963	7.512778701454
14	6.016 639 365 097	7.136 449 095 154	6.603 227 003 011	7.872.998 747 258
15	6.351 612 912 105	7.452 756 727 145	•	
16	6.658 720 495 811	7.757 175 840 949		
17	6.983 036 971 627	8.062 461 937 377		
18	7.283 785 190 542	8.357 641 548 941		

Table 4. Estimates of v in two dimensions for several values of the strength parameter u.

ν
0.485 ± 0.005
0.46 ± 0.01
0.40 ± 0.01
0.34 ± 0.01
0.29 ± 0.01
0.26 ± 0.03

We observe a decreasing of ν , faster than in one dimension, when *u* decreases. This result is also different from the behaviour of the static model of Stanley *et al*, where the mean-square displacement $\langle R_N^2 \rangle$ saturates in two and three dimensions [8].



Figure 7. Plot of $s_N^{(1)} \times 1/N$ (equation (12b)) for u = -0.5 and u = -1.0 in the square (\Box) and the triangular (Δ) lattices. The empty polygons correspond to u = -0.5 and the full ones to u = -1.0.

In figure 7 we plot $s_N^{(1)} \times 1/N$ (equation (12b)) for u = -0.5 and -1.0, in the square and the triangular lattice. For RW it is expected that [1]

$$\langle S_N \rangle \sim N/\log(N) \qquad N \to \infty$$
 (13)

then the differences in figure 7 may appear due to non-algebraic corrections in the asymptotic form of $\langle S_N \rangle$. When we substitute $\langle S_N \rangle$ for $\langle S_N \rangle \log N$ in μ_N (equation (10b)), the plots of $s_N^{(1)} \times 1/N$ for those lattices also have differences in all orders N. So the non-algebraic corrections must be more complicated than the one of RW, and suitable techniques of series analysis would be necessary to find the correct asymptotic form. As the exponent ν depends on the parameter u, these corrections may also depend on it.

Sapozhnikov [13] found v = 0.38 for u = -1.0 and v = 0.32 for u = -2.0 in his simulations. These results are good when compared to ours. For u = -0.5 he obtained v = 0.49 and proposed that there is a critical value u_c so that $v = \frac{1}{2}$ for $0 < u < u_c$. However, our data indicate a continuous variation of v even for small u, so that proposal is discarded.

5. SATW in three and four dimensions

The series for the simple cubic lattice were calculated up to N = 14, for *u* ranging from -0.2 to -1.5. As the series are short and the oscillations increase with |u|, it is not possible to obtain accurate estimates of the exponents for higher values of that parameter.

We plot $\nu_N^{(1)} \times 1/N$ for u = -1.0 in figure 8. It is clear that SATW displays anomalous diffusion in this lattice. This result in three dimensions is interesting for a comparison with data from real systems. In table 5 we show the final estimates of ν in three dimensions. It decreases with u as before, but not as quickly as in two dimensions.

The proposal of Sapozhnikov [13] that $\frac{1}{4} < \nu < \frac{1}{3}$ in three dimensions is discarded by our results, and they are very distant of the saturation effect in the corresponding static model [8].

Table 5. Estimates of v and s in three dimensions for several values of the strength parameter u,

u	ν	5	
-0.2	0.50 ± 0.01	0.945 ± 0.010	
-0.5	0.485 ± 0.015	0.93 ± 0.02	
-1.0	0.45 ± 0.02	0.88 ± 0.02	
-1.5	0.39 ± 0.02	0.825 ± 0.025	



Figure 8. Plot of $v_N^{(1)} \times 1/N$ (equation (12*a*)) for u = -1.0 in the simple cubic lattice.



Figure 9. Plot of $v_N^{(1)} \times 1/N$ (equation (12a)) for u = -1.5 in the four-dimensional hypercubic lattice.

We also show in table 5 the final estimates for exponent s (equation (5)). For RW, s = 1 in three or more dimensions [1], and for SATW s seems to decrease continuously when u decreases.

In four dimensions, anomalous diffusion for SATW is also observed. We calculated series up to N = 12 in a hypercubic lattice for u = -0.5, -1.0 and -1.5, and for the last value we estimate $v = 0.44 \pm 0.02$ (see the plot of $v_N^{(1)} \times 1/N$ in figure 9), which certainly means that $v < \frac{1}{2}$.

It is also observed that s < 1 in four dimensions. For u = -1.5, we estimate $s = 0.895 \pm 0.025$.

When the dimension is increased from 2 to 4, the decreasing of v and s with the parameter u is slower. For the model of Stanley *et al* a saturation of $\langle R_N^2 \rangle$ is observed in $D \ge 2$, but the very opposite occurs with SATW. It seems that we are moving towards the upper critical dimension D_c of SATW, where we expect $v = \frac{1}{2}$ and s = 1 for all u (the RW values). Our results show that $D_c > 4$, but we are not able to decide whether D_c is finite or not.

6. Summary and discussion

SATW was studied in dimensions from one to four using exact enumeration techniques. Approximations of exponents v (equation (1)) and s (equation (5)) were found for several values of the parameter u (< 0), with |u| measuring the strength of attraction.

In all dimensions it displays anomalous diffusion and the exponents decrease continuously with u. This non-universal behaviour is very important when SATW is compared with previously studied models of generalized random walks, static [11] or dynamic [12]. For those systems, non-universal exponents were found by changing the power α according to which different visits to a site were weighted (equation (2)), but not by changing the strength parameter. Furthermore, most of those results were limited to one dimension, while SATW keeps its interesting properties in a large range of spacial dimensions. Then the estimates presented here for two and especially for three dimensions may be useful from an experimental point of view.

It was already pointed out that, in the energy-entropy balance of interacting random walk models, the local normalization condition favours the entropic term, while global normalization favours the energetic term [10]. We found exponents ν for SATW (tables 2, 4 and 5) in all dimensions greater than the exponents ν of the corresponding static model [8] $(\nu = \frac{1}{3} \text{ in } D = 1, \nu = 0 \text{ in } D \ge 2)$. This is the expected behaviour since the entropic term favours $\nu \rightarrow \frac{1}{2}$ (RW) and the energetic term, in case of attraction, favours $\nu \rightarrow 0$ (collapse). According to this analysis and the results of section 3, in one dimension we expect $\nu \rightarrow \frac{1}{3}$ for SATW when $|u| \rightarrow \infty$. In $2 \le D \le D_c$ we expect $\nu \rightarrow 0$ for $|u| \rightarrow \infty$.

New perspectives are opened by our results. More accurate estimates of exponents ν and s, obtained from longer series or from simulations, may describe the influence of the parameter u quantitatively, bringing new informations about the universality classes of SATW. If this work is done in dimensions greater than four, it could help to find the upper critial dimension. Finally, the results presented here motivate the proposal and study of different generalized random walk models that may display interesting features and represent the behaviour of real systems. Work along these lines is in progress.

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