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On self-repelling walks

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Abstract. We investigate the properties of self-repelling walks—otherwise known as 'true' self-avoiding walks—in both one and two dimensions for a range of values of the repulsion parameter g, $0.2 \leq g \leq 10.0$. In one dimension we have obtained 24 terms of the generating function of the mean-square end-to-end distance $\langle R_N^2 \rangle$, while on the two-dimensional square lattice we have obtained 12-15 terms. In one dimension we find the data to be well fitted by $\langle R_N^2 \rangle = N^{4/3}(A + B/N^{1/3} + C/N + O(1/N))$ and in two dimensions by $\langle R_N^2 \rangle = DN|\ln N|^{\alpha}(1 + O(\ln|\ln N|/\ln N))$ with $\alpha \approx 0.5$. Estimates of the amplitudes A and D are also obtained.

1. Introduction

A new and interesting variation of self-avoiding walks was recently proposed by Amit *et al* (1983). This variation was named the 'true' self-avoiding walk (TSAW) to distinguish it from the usual self-avoiding walk (SAW). We consider this name quite inappropriate on the semantic grounds that anything called a '*true*' *self-avoiding walk* has a moral obligation to be self avoiding. In fact, TSAWs may recross themselves with non-zero probability, unlike SAWs, which are truly self avoiding. Accordingly, we suggest the name 'self-repelling walk' (SRW) as semantically appropriate.

On a d-dimensional hypercubic lattice an SRW may visit *any* site i adjacent to its current end point with probability p_i, which depends on the number of times site i has been visited previously, denoted n_i, and the repulsion $g > 0$, through the relation

$$p_i = \exp(-gn_i)\left(\sum_{i=1}^{2d} \exp(-gn_i)\right)^{-1}. \tag{1.1}$$

The probability of a given walk is just the product of the probabilities of the N steps. Like the SAW problem, the SRW problem is also a non-Markovian process.

Note too that all $(2d)^N$ N-step pure random walks are possible (with varying probability) so that the chain generating function (CGF) is just $C(x) = 1/(1-2dx)$, a rather uninteresting quantity. Weighting each SRW by its probability just modifies this quantity to give the even less interesting result for the weighted CGF $C_W(x) = 1/(1-x)$.

In one dimension, the parameter g effectively interpolates between the SAW ($g = \infty$) and the pure random walks ($g = 0$). The interpolation is discontinuous as the critical exponents are those appropriate to SRWs for finite g and become SAW-like only for $g = \infty$. In higher dimensions, however, the $g \to \infty$ limit does *not* correspond to SAWs as is demonstrated explicitly by Amit *et al*, though of course $g = 0$ still corresponds to the pure random walk.

Amit *et al* also showed that the critical dimensionality of this model is $d_c = 2$, quite different from the result $d_c = 4$ which holds for SAWs. A renormalisation group (RG) calculation gave

$$\langle R_N^2 \rangle \sim AN(\ln N)^{0.4}(1 + B \ln|\ln N|/\ln N) \qquad \text{for } d = d_c = 2.$$

A Monte Carlo study of two-dimensional SRWs for $g = 0.1$, 0.3 and 1.0 supported this form.

In dimensions below the critical dimension Amit *et al* do not derive critical exponents, but from their results $\beta = -\frac{1}{2}\varepsilon u + \frac{5}{4}u^2$, $u^* = \frac{2}{5}\varepsilon$ and $\gamma = \frac{1}{2}u^* = \frac{1}{5}\varepsilon$ one may conclude $\langle R_N^2 \rangle \sim N^{6\varepsilon/5}$ or

$$\langle R_N^2 \rangle \sim N^{6/5}$$

to first order in ε for $\varepsilon = d = 1$. Subsequently Pietronero (1983) advanced a Flory-type argument that yielded $\nu = \frac{1}{2}$ for $d \geq d_c = 2$ and $\nu = 2/(2+d)$ for $d < 2$ when ν is the exponent characterising $\langle R_N^2 \rangle$ through $\langle R_N^2 \rangle \sim N^{2\nu}$. Pietronero argued that this result is inapplicable at $d = 1$, $g = \infty$ for which $\nu = 1$ holds. Subsequently Obukhov (1984) argued from a small-g expansion that Pietronero's result holds explicitly at $d = 1$, giving $\nu = \frac{2}{3}$ for $0 < g < \infty$.

More recently, Rammal *et al* (1984) have carried out a Monte Carlo study on the one-dimensional SRW problem and find $\nu \approx \frac{2}{3}$. They also consider the case $g < 0$ and find a saturation effect so that $\lim_{N\to\infty} \langle R_N^2 \rangle = R_\infty^2(g) < \infty$ for $g < 0$ (this case could be called the self-attracting walk). de Queiroz *et al* (1984) considered the crossover behaviour as $g \to 0$ and $g \to \infty$. From a real-space RG analysis they provide convincing evidence of a value for ν different from both the SAW and random-walk values, and constant for $0 < g < \infty$.

Since the completion of this work we have received a preprint from Stella *et al* (1984) who generate series expansions for one-dimensional SRWs and find $\nu = 0.67 \pm 0.04$, in agreement with both Monte Carlo results and our results. Another recent paper by Family and Daoud (1984) provides a Flory theory for SRWs, yielding $\nu = 2/(d+2)$ for $d \leq d_c = 2$, and argues that the SRW models the *statistics* of a linear polymer in a polydispersed solution.

In this paper we have studied the SRW in both one and two dimensions by generating series expansions for $\langle R_N^2 \rangle$ for $N \leq 24$ ($d = 1$) and $N \leq 15$ ($d = 2$) for $0.2 \leq g \leq 10.0$.

2. One-dimensional results

In table 1 we show the coefficients $\langle R_N^2 \rangle$ for $1 \leq N \leq 24$ for several values of g in the range $0.2 \leq g \leq 10.0$. For large g, it is clear that $\langle R_N^2 \rangle \approx N^2$, and the maximum value of N we have used ($N_{max} = 24$) is far too small for asymptotic behaviour to be evident. Indeed, the Monte Carlo results of Rammal *et al* show that, for $g = 10$, deviations from $\langle R_N^2 \rangle \sim N^2$ require $N \geq 500$ in order to be evident. Thus our analysis will focus on lower values of g, which we restrict to $g \leq 2.0$. The heuristic arguments of Amit *et al*, while giving the wrong exponent, do suggest that the correct form for $\langle R_N^2 \rangle$ should contain at least two terms, one corresponding to the random-walk behaviour ($\propto N$) appropriate to $g = 0$ and the other ($\propto N^{4/3}$) appropriate to $g > 0$. Accordingly we write

$$\langle R_N^2 \rangle \sim N^{4/3}(A + B/N^{1/3} + C/N + D/N^{4/3} + \ldots). \tag{2.1}$$

Table 1. Mean-square end-to-end distances for one-dimensional self-repelling walks.

N	$g=0.2$	$g=0.5$	$g=\ln 2$	$g=1.0$	$g=2.0$	$g=5.0$	$g=10.0$
1	1.000 00	1.000 00	1.000 00	1.000 00	1.000 00	1.000 00	1.000 00
2	2.199 34	2.489 84	2.666 67	2.924 23	3.523 19	3.973 23	3.999 82
3	3.418 54	4.099 65	4.555 56	5.275 57	7.206 43	8.893 27	8.999 27
4	4.777 03	6.017 95	6.844 44	8.167 08	11.981 34	15.747 37	15.998 27
5	6.162 14	8.068 62	9.351 61	11.425 18	24.715 01	24.522 57	24.996 73
6	7.657 66	10.364 41	12.188 31	15.149 39	24.394 41	35.206 55	35.994 55
7	9.178 83	12.765 53	15.189 74	19.150 81	31.879 56	47.786 43	48.991 65
8	10.794 73	15.382 19	18.479 33	23.546 09	40.163 59	62.250 02	63.987 93
9	12.433 74	18.088 86	21.912 76	28.183 09	49.133 39	78.584 64	80.983 30
10	14.157 05	20.984 33	25.593 65	33.155 40	58.790 55	96.778 27	99.977 67
11	15.901 54	23.963 55	29.407 73	38.344 56	69.037 24	116.818 37	120.970 95
12	17.722 31	27.109 98	33.440 57	43.830 54	79.884 29	138.693 18	143.963 06
13	19.563 05	30.334 93	37.595 38	49.510 95	91.244 87	162.390 27	168.953 89
14	21.473 59	33.711 36	41.948 61	55.459 76	103.136 94	187.898 10	195.943 36
15	23.403 28	37.161 23	46.414 62	61.587 10	115.482 83	215.204 41	224.931 38
16	25.397 45	40.750 30	51.062 07	67.957 82	128.303 24	244.297 81	255.917 85
17	27.410 13	44.408 59	55.815 32	74.494 50	141.529 45	275.166 23	288.902 68
18	29.482 89	48.195 80	60.735 84	81.255 04	155.185 03	307.798 49	323.885 80
19	31.573 57	52.048 77	65.756 03	88.169 61	169.205 95	342.182 62	360.867 13
20	33.720 66	56.021 98	70.931 90	95.292 34	183.619 09	378.307 68	399.846 50
21	35.885 14	60.057 91	76.201 87	102.558 88	198.364 96	416.161 87	440.823 91
22	38.102 87	64.206 72	81.617 78	110.019 93	213.471 05	455.734 41	483 799 22
23	40.337 52	68.415 49	87.122 86	117.616 20	228.882 98	497.013 58	528.772 34
24	42.622 69	72.730 83	92.765 48	125.395 08	244.628 60	539.988 89	575.743 23

By fitting our data to the form (2.1) we find a consistent picture emerges. To be precise, we have solved (2.1) first by truncating at the $O(N^{-1})$ and then at the $O(N^{-4/3})$ term. In order to remove the characteristic odd–even oscillation of hypercubic lattice data, we have transformed our series using the transformation (Watts 1974) $z=20x/(9x+11)$ where x is the expansion variable in the original generating function $R^2(x)=\Sigma_{N>0}\langle R_N^2\rangle x^N$. This transformation maps the critical point $x_c=1$ to $z_c=1$, but maps the 'antiferromagnetic' critical point $x=-1$ to $z=-10$, far enough away from the radius of convergence that its effect is negligible. After transformation, we denote the transformed quantity by

$$\langle \tilde{R}_N^2\rangle = N^{4/3}(\tilde{A}+\tilde{B}/N^{1/3}+\tilde{C}/N+\tilde{D}/N^{4/3}+\ldots) \tag{2.2}$$

where $\tilde{A}=A(0.55)^{2\nu+1}=0.247\,84A$.

We find that truncating the series (2.2) after the term $\tilde{C}/N$ gives a very satisfactory fit. The next term, $\tilde{D}/N^{4/3}$, in fact slightly improves the quality of the fit, while not significantly changing the leading amplitude $\tilde{A}$. In table 2 we show the results of our analysis for a representative value of g, $g=\ln 2$, where successive triplets of terms from the transformed series $\langle \tilde{R}_N^2\rangle$, $\langle \tilde{R}_{N-1}^2\rangle$ and $\langle \tilde{R}_{N-2}^2\rangle$ are used to find $\tilde{A}$, $\tilde{B}$ and $\tilde{C}$ in (2.2), and successive quadruplets of terms are used to fit to $\tilde{A}$, $\tilde{B}$, $\tilde{C}$ and $\tilde{D}$.

We have extrapolated the sequence of estimates for the leading amplitude $\tilde{A}$ for all values of g used, and find the results for A shown in table 3. Our estimates encompass both sets of results shown in table 2. Because the amplitudes of the

Table 2. Results of fitting the transformed data of table 1 to the form (2.2) ($g = \ln 2$).

N	$\tilde{A}$	$\tilde{B}$	$\tilde{C}$	$\tilde{A}$	$\tilde{B}$	$\tilde{C}$	$\tilde{D}$
10	0.4322	−0.4000	0.6728	0.4931	−0.6532	1.7653	−1.1339
11	0.4412	−0.4286	0.7155	0.5005	−0.6840	1.8984	−1.2720
12	0.4490	−0.4543	0.7566	0.5064	−0.7094	2.0158	−1.3983
13	0.4559	−0.4775	0.7958	0.5111	−0.7304	2.1196	−1.5135
14	0.4619	−0.4984	0.8334	0.5150	−0.7482	2.2129	−1.6203
15	0.4672	−0.5174	0.8693	0.5183	−0.7636	2.2975	−1.7197
16	0.4719	−0.5348	0.9037	0.5210	−0.7767	2.3740	−1.8117
17	0.4762	−0.5506	0.9366	0.5233	−0.7881	2.4427	−1.8964
18	0.4800	−0.5652	0.9680	0.5252	−0.7978	2.5044	−1.9741
19	0.4834	−0.5786	0.9982	0.5269	−0.8061	2.5595	−2.0448
20	0.4866	−0.5910	1.0270	0.5282	−0.8132	2.6082	−2.1087
21	0.4894	−0.6024	1.0546	0.5293	−0.8192	2.6509	−2.1655
22	0.4920	−0.6130	1.0810	0.5302	−0.8242	2.6874	−2.2152
23	0.4943	−0.6228	1.1063	0.5310	−0.8282	2.7180	−2.2573
24	0.4965	−0.6319	1.1304	0.5315	−0.8313	2.7426	−2.2917

Table 3. Leading amplitudes for one-dimensional self-repelling walks.

g	A
0.2	0.18 ± 0.03
0.5	0.42 ± 0.03
ln 2	0.54 ± 0.05
1.0	0.72 ± 0.06
2.0	1.3 ± 0.3

correction terms depend significantly on the set of results used in table 2—that is, on whether we are fitting to three or four parameters in (2.2)—we provide no estimate for these amplitudes. However it is clear from our analysis that $\tilde{B}$ is (algebraically) decreasing as g increases, while the behaviour of $\tilde{C}$ is not monotonic in g.

We have also investigated an alternative form to (2.1) and (2.2) in which we include an additional term proportional to $N^{-2/3}$. This reflects the possibility that, if there is a 'correction-to-scaling' exponent $\Delta_1 = \frac{1}{3}$, then there is a second 'correction-to-scaling' exponent of $\Delta_2 = \frac{2}{3}$. That is, we assume that

$$\langle R_N^2 \rangle / N^{4/3} = \sum_{k \geq 0} a_k / N^{k/3}. \tag{2.3}$$

The apparent convergence of the amplitudes a_k is found to be somewhat less rapid and consistent than that obtained from the assumed form (2.1) and (2.2). Under this alternative assumption the leading amplitude is between 1% and 10% higher than that given in table 3, for different values of g, though in all cases within the error limits quoted.

Thus we conclude that we cannot unequivocally distinguish between (2.1) and (2.3), though the analysis favours (2.1) somewhat. In either event, table 3 contains estimates of the critical amplitudes.

Table 4. Mean square end-to-end distances for two-dimensional self-repelling walks.

N	$g=0.2$	$g=0.5$	$g=\ln 2$	$g=1.0$	$g=2.0$	$g=5.0$	$g=10.0$
1	1.000 00	1.000 00	1.000 00	1.000 00	1.000 00	1.000 00	1.000 00
2	2.094 94	2.218 20	2.285 71	2.375 38	2.551 56	2.660 69	2.666 63
3	3.194 38	3.460 20	3.612 24	3.821 22	4.255 23	4.539 64	4.555 45
4	4.342 39	4.801 91	5.063 02	5.423 16	6.188 63	6.710 93	6.740 54
5	5.494 56	6.161 64	6.541 37	7.065 89	8.186 16	8.955 95	8.999 70
6	6.678 41	7.583 79	8.096 74	8.804 29	10.318 90	11.367 73	11.427 58
7	7.865 41	9.017 75	9.669 06	10.565 96	12.480 86	13.797 40	13.871 92
8	9.075 74	10.496 74	11.296 53	12.395 52	14.738 54	16.349 57	16.440 62
9	10.288 48	11.984 10	12.935 77	14.240 95	17.015 81	18.911 14	19.017 34
10	11.519 58	13.506 33	14.617 40	16.138 01	19.363 41	21.561 27	21.684 08
11	12.752 61	15.035 05	16.308 12	18.047 37	21.727 04	24.222 64	24.361 30
12	14.000 71	16.591 99	18.032 93	19.997 91	24.145 79	26.952 35	27.107 90
13	15.250 42	18.154 27					29.864 22
14	16.512 87	19.740 13					32.678 56
15		21.330 53					

3. Two-dimensional results

In table 4 we show our data for $\langle R_N^2\rangle$ for the two-dimensional series for $1\leqslant N\leqslant 15$ and $0.2\leqslant g\leqslant 10$. The RG calculations of Amit *et al* suggested asymptotic behaviour of the form

$$\langle R_N^2\rangle \sim N(\ln N)^\alpha(D+E\ \ln|\ln N|/\ln N) \tag{3.1}$$

with $\alpha=0.4$. Subsequently Obukhov and Peliti (1983) disputed this result on the grounds that the calculation of Amit *et al* assumed that only one coupling constant needed renormalisation in order to remove all infinities in the perturbation theory, while they found that at least two and possibly three coupling constants are involved. As a consequence, with two coupling constants involved, they found $\alpha=1.0$. They also make the point that this value of α will manifest itself earlier—that is for lower N values—the larger the value of g. Indeed, for $g=\infty$ Amit *et al* did extract a small number of walks in their Monte Carlo study which better fitted the form $\langle R_N^2\rangle\sim N\ln N$.

We have investigated this disagreement by analysing our series data as discussed below. Note however that the correction term in (3.1) is very slowly varying, and is essentially undetectable by series analysis methods with our range of N values. As N ranges from 10 to 20, the correction term ranges from $0.362E$ to $0.366E$. Thus we expect an 'effective' amplitude of $(D+0.36E)$.

To estimate α, we first form the sequence

$$s_N=\{\ln[(\langle R_N^2\rangle/N)/(\langle R_{N-2}^2\rangle/(N-2))]\}/\ln(\ln N/\ln(N-2)). \tag{3.2}$$

If $\langle R_N^2\rangle\sim DN(\ln N)^\alpha$, then $s_N\sim\alpha$. The sequence $\{s_N\}$ is defined using alternate terms in $\langle R_N^2\rangle$ in order to accommodate the oscillation discussed previously, and the sequence $\{t_N\}$ and $\{u_N\}$, defined by

$$\begin{aligned} t_N&=\tfrac{1}{2}[Ns_N-(N-2)s_{N-2}]\\ u_N&=[N^2t_N-(N-2)^2t_{N-2}]/(4N-4), \end{aligned} \tag{3.3}$$

Table 5. Direct estimates (s_N), linear (t_N) and quadratic (u_N) extrapolants of the confluent logarithmic exponent α for two-dimensional self-repelling walks.

	$g=0.2$			$g=0.5$			$g=1$			$g=5$			$g=10$		
N	s_N	t_N	u_N	s_N	t_N	u_N	s_N	t_N	u_N	s_N	t_N	u_N	s_N	t_N	u_N
6	0.097	0.189		0.201	0.374		0.308	0.543		0.474	0.752		0.477	0.756	
7	0.117	0.204		0.234	0.385		0.347	0.535		0.504	0.660		0.507	0.660	
8	0.128	0.219	0.258	0.251	0.401	0.436	0.365	0.537	0.529	0.509	0.613	0.434	0.511	0.611	0.425
9	0.142	0.228	0.266	0.272	0.407	0.441	0.388	0.533	0.530	0.527	0.605	0.521	0.528	0.604	0.517
10	0.150	0.239	0.274	0.284	0.416	0.443	0.399	0.515	0.531	0.525	0.592	0.555	0.527	0.590	0.533
11	0.161	0.245	0.279	0.299	0.419	0.444	0.414	0.531	0.528	0.536	0.580	0.529	0.537	0.579	0.528
12	0.167	0.252	0.283	0.308	0.426	0.447	0.422	0.533	0.530	0.536	0.590	0.583	0.537	0.589	0.587
13	0.175	0.257	0.287	0.319	0.427	0.448							0.544	0.577	0.574
14	0.181	0.263	0.291	0.325	0.432	0.450							0.544	0.586	0.576
15				0.334	0.433	0.450									

extropolate alternate s_N's against $1/N$ and $1/N^2$, in the usual manner of the ratio method. These sequences are shown in table 5, and it can be seen that for $g = 0.2$ a rapidly increasing sequence of estimates suggests $\alpha > 0.3$. For $g = 0.5$ the rate of increase has substantially declined, and supports $\alpha \geqslant 0.45$. For $g = 1$ the estimates are quite steady around $\alpha \approx 0.53$, while for $g = 5$ and $g = 10$ the estimates are generally decreasing, suggesting $\alpha \leqslant 0.6$. Thus for all values of g we have used we find consistent evidence of $\alpha \approx \frac{1}{2}$. This is much closer to the result of Amit *et al* ($\alpha = 0.4$) than that of Obukhov and Peliti ($\alpha = 1.0$). It can of course be argued that our series are short, with $N_{max} = 15$, and that asymptotic behaviour only manifests itself for larger values of N. Such an objection is entirely valid, but not totally convincing. Firstly, it would be surprising if *all* values of g pointed to the same (erroneous) value of α, and it *is* the case that a value of $\alpha \approx \frac{1}{2}$ is indicated by all the series. Secondly, for the self-avoiding walk at the critical dimension ($d = d_c = 4$), a similar number of terms has been shown to be adequate (Guttmann 1978) to determine the correct confluent logarithmic exponent.

It seems worthwhile to conduct a thorough Monte Carlo analysis in order to resolve this point. For intermediate values of g, that is $g \approx 1$, the Monte Carlo data of Amit *et al* with step size up to $N \approx 2^{14} \approx 16\,000$ favours $\alpha = 0.4$ over $\alpha = 1.0$, so clearly very large values of N indeed will be needed if this value of α is incorrect. (However, Obukhov and Peliti reanalyse the data of Amit *et al* at $g = 10$ and find support for $\alpha = 1.0$.)

We have also estimated the effective critical amplitude by forming the sequence $D_N = \langle R_N^2 \rangle / N(\ln N)^\alpha$ with $\alpha = 0.5$. Extrapolating alternate terms in the sequence $\{D_N\}$ both linearly and quadratically against $1/N$, as was done to estimate α, we find the following values of the effective amplitude: 0.62 ($g = 0.2$), 0.81 ($g = 0.5$), 0.90 ($g = \ln 2$), 1.04 ($g = 1.0$), 1.4 ($g = 5$) and 1.4 ($g = 10.0$). These values depend on the value of α, and included possibly substantial contributions from slowly varying correction terms, so their values should not be uncritically accepted. The trend of increasing amplitude with increasing g value, approaching a positive asymptote as $g \to \infty$, is likely to be correct however. From the Monte Carlo plots of Amit *et al*, which assume $\alpha = 0.4$, we find for the amplitudes 0.43 ($g = 0.1$), 0.61 ($g = 0.3$) and 1.05 ($g = 1.0$) in reasonable agreement with our own results. Note that natural logarithms are used throughout this paper, whereas some workers use $\log_2$.

4. Conclusion

We find that the mean-square lengths of one-dimensional SRWs are well fitted by (2.1) which implies a correction-to-scaling exponent of $\Delta = \frac{1}{3}$ for all g. The critical amplitude A is found to be an increasing function of g, and we see that A/g is a decreasing function of g, within the range of g values used. This is consistent with the 'small-g' approximation of Obukhov (1984) who gives $A \sim g^{2/3}$ *for small* g. An alternative form for $\langle R_N^2 \rangle$ is given by (2.3), and it is found that this does not fit the data quite as well as (2.1), but does not significantly alter the amplitude estimates.

For two-dimensional SRWs we find that the mean-square lengths are well fitted by (3.1), with confluent logarithmic exponent $\alpha \approx 0.5$, in reasonable agreement with the earlier work of Amit *et al*, rather than the later theory of Obukhov and Peliti. The qualitative behaviour of the critical amplitude is the same as that for one-dimensional walks discussed above.

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