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LETTER TO THE EDITOR

Asymptotic properties of spiral self-avoiding walks

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Abstract. We consider the spiral self-avoiding walk model recently introduced by Privman. On the basis of an analogy with the partitioning of the integers, we argue that the number of N-step spiral walks should increase asymptotically as $\rho^{\sqrt{N}}$ with ρ a constant, leading to an essential singularity in the generating function. Enumeration data to 65 terms indicates, however, that c_N apparently varies as ρ^{N^α}, with $\alpha \simeq 0.55$. We also study the N-dependence of the mean-square end-to-end distance, $\langle R_N^2 \rangle$, and of the mean rotation angle, $\langle \theta N \rangle$, for N-step walks. From series extrapolations, we estimate that $\langle R_N^2 \rangle \sim N^{1.2}$, and $\langle \theta_N \rangle \sim N^{0.55}$.

Very recently, Privman (1983) introduced for the square lattice a 'spiral' self-avoiding walk (SAW) model, defined to be a SAW with the additional constraint that a 90° left-hand turn is not allowed. Accordingly, a walk will tend to spiral around the origin in the clockwise sense (figure 1). On the basis of exact enumeration data to order 40, Privman argued that the spiral SAW model is in a different universality class than the isotropic SAW problem. This result was interpreted as arising from the fact that the spiral restriction is effectively global in nature when it augments the self-avoiding constraint.

Well known examples of a global constraint modifying the universality class occur in 'directed' problems (see e.g. Kinzel 1983). The directionality constraint can be thought of as analogous to a uniform drift superimposed on a transport problem. This

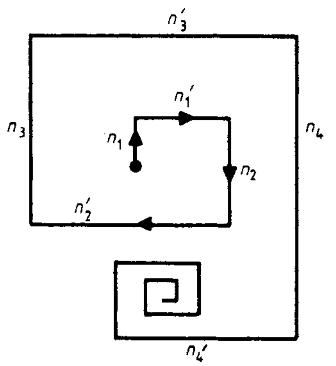

Figure 1. Schematic picture of a spiral SAW on the square lattice. The lengths of the vertical segments are denoted by $n_1, n_2, \ldots$, and the horizontal segments by $n_1', n_2', \ldots$.

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drift may be accounted for by a term of the form $\boldsymbol{v}_{\text{drift}} \cdot \boldsymbol{k}$ in a mean-field propagator, where $\boldsymbol{k}$ is the wave vector (see e.g., Redner 1982). The presence of this term is sufficient to understand the essential anisotropic nature of directed problems. Similarly, one may regard the spiral problem as a critical phonomenon taking place in a rotational flow field. Such an effect might be accounted for at the mean-field level by including a term of the form $\boldsymbol{\omega} \times \boldsymbol{k}$ in the propagator, where $\boldsymbol{\omega}$ is a rotational velocity. Such a term, linear in $\boldsymbol{k}$, should also modify the large-distance behaviour of the model. These observations also suggest that the average rotation angle of spiral walks will possess an interesting asymptotic behaviour.

In this letter, we present evidence which indicates that spiral self-avoiding walks exhibit a novel critical behaviour. By making an analogy with the problem of the 'partitioning' of integers, we argue that the number of N-step walks, c_N, should grow as $\rho^{\sqrt{N}}$, with ρ a constant, leading to an essential singularity in the associated generating function $G(x) = \Sigma_N c_N x^N$. This is in sharp contrast to the usual SAW model where $c_N \sim \mu^N N^{\gamma-1}$, so that $G(x)$ possesses the power law singularity $(x - x_c)^{-\gamma}$. To test this possibility, we extend the series data of Privman to order 65. Extrapolation of the series indicates, however, that the growth law for the c_N is $c_N \sim \rho^{N^\alpha}$, with $\alpha \simeq 0.55$. We also examine the N-dependence of the mean-square end to end distance, $\langle R_N^2 \rangle$, and the mean rotation angle with respect to the starting direction, $\langle \theta_N \rangle$. On the basis of extrapolating 65 and 60 term series respectively, it appears that these two quantities exhibit the following power-law dependences: $\langle R_N^2 \rangle \sim N^{2\nu}$ with $\nu \simeq 0.60$, and $\langle \theta_N \rangle \sim N^{\nu_\theta}$ with $\nu_\theta \simeq 0.55$.

In table 1, we present the enumeration data of spiral walks with the starting direction fixed. The enumeration for c_N and $\langle R_N^2 \rangle$ to order 65 and for $\langle \theta_N \rangle$ to order 60 require approximately 5.5 h and 6.1 h of CPU time respectively on an IBM 3081-D machine. The series were obtained by a direct enumeration of all walks, and relatively lengthy series were obtainable due to the slow growth rate of the c_N on N. For the purposes of extrapolation, the ratio method appears to be the simplest and best-suited to detect the asymptotic behaviour. Figure 2 shows the results of extrapolations for the critical point based on fitting c_N to $\mu^N N^{\gamma-1}$. One observes that the sequence of critical point extrapolants based on even series terms and the one based on the odd terms show contradictory trends. A rough visual extrapolation suggests $\mu \simeq 1.04$, although it seems possible that the value $\mu = 1$ might result if there were considerably more terms

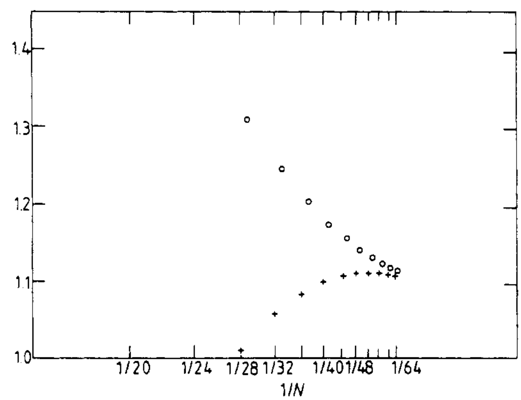

Figure 2. Ratio extrapolants for the critical point plotted against $1/N$: even terms (+), and odd terms (O).

Table 1. Enumeration data for spiral SAWs; the last digit after the decimal may be rounded off.

N	c_N	$\langle R_N^2\rangle$	$\langle\theta_N\rangle$	N	c_N	$\langle R_N^2\rangle$	$\langle\theta_N\rangle$
1	1	1.0000	0.0000	36	689 678	66.7302	5.5637
2	2	3.0000	0.3927	37	893 884	68.9894	5.6593
3	4	5.0000	0.7854	38	1 153 837	71.3421	5.7541
4	7	7.4286	1.0098	39	1 486 445	73.6470	5.8474
5	13	9.0000	1.3291	40	1 908 002	76.0297	5.9399
6	21	11.4286	1.4960	41	2 444 270	78.3747	6.0309
7	37	12.4595	1.7831	42	3 121 064	80.7849	6.1213
8	57	14.8070	1.9290	43	3 977 420	83.1648	6.2103
9	95	15.6526	2.1660	44	5 053 839	85.5996	6.2986
10	143	17.8182	2.3177	45	6 409 117	88.0105	6.3858
11	227	18.7269	2.5119	46	8 106 019	90.4675	6.4722
12	335	20.7761	2.6633	47	10 232 851	92.9058	6.5576
13	513	21.8031	2.8323	48	12 885 792	95.3831	6.6422
14	744	23.7930	2.9801	49	16 196 772	97.8457	6.7259
15	1 106	24.9783	3.1317	50	20 312 050	100.3418	6.8089
16	1 580	26.9519	3.2728	51	25 427 666	102.8265	6.8911
17	2 294	28.2816	3.4141	52	31 764 104	105.3400	6.9725
18	3 232	30.2661	3.5489	53	39 611 552	107.8451	7.0531
19	4 600	31.7461	3.6804	54	49 299 720	110.3751	7.1331
20	6 402	33.7470	3.8102	55	61 256 038	112.8992	7.2123
21	8 962	35.3584	3.9351	56	75 970 439	115.4453	7.2909
22	12 329	37.3959	4.0586	57	94 069 393	117.9875	7.3688
23	17 019	39.1212	4.1785	58	116 276 080	120.5492	7.4460
24	23 169	41.1990	4.2969	59	143 504 932	123.1090	7.5226
25	31 589	43.0293	4.4118	60	176 816 714	125.6863	7.5986
26	42 599	45.1472	4.5260	61	217 540 090	128.2633	
27	57 453	47.0724	4.6367	62	267 222 691	130.8562	
28	76 796	49.2329	4.7468	63	327 786 359	133.4502	
29	102 588	51.2410	4.8540	64	401 476 801	136.0590	
30	136 019	53.4446	4.9604	65	491 062 665	138.6701	
31	180 131	55.5269	5.0642				
32	237 061	57.7712	5.1673				
33	311 489	59.9202	5.2681				
34	407 097	62.2032	5.3683				
35	531 113	64.4108	5.4664				

available for analysis. Moreover, the estimate for γ is approximately 7 by order 65, and it is still increasing steadily with N, suggesting that the extrapolated value may be infinite.

These observations suggest that the assumption $c_N \sim \mu^N N^{\gamma-1}$ is not valid for spiral self-avoiding walks, and that one should seek an alternative law for the c_N. Our approach for finding the N-dependence of c_N, is based on examining figure 1. We denote the number of bonds in the successive vertical segments by $n_1, n_2, \ldots$, and the number in the horizontal segments by $n_1', n_2', \ldots$. As long as $n_1 < n_2 < \ldots$ and $n_1' < n_2' < \ldots$ the walk can continue to grow. If, however, one of the inequalities is not satisfied for some n_k, then the walk must eventually 'die' in a finite vortex. Thus one might expect that the asymptotic behaviour of the c_N to be dominated by only those walks which satisfy the above inequalities.

These inequalities define a partitioning problem where the total number of vertical steps in the walk, N_{vert}, may be divided into k separate segments of unequal and increasing size (except that the last segment may have arbitrary length). A similar situation occurs for the horizontal bonds, so that c_N is essentially given by the total number of these partitionings for all possible values of N_{vert} and N_{horiz} subject to $N_{\text{vert}}+N_{\text{horiz}}=N$. The partitioning of the integers is a classical problem, and the results relevant to the spiral SAW model are well known (see e.g., Abramowitz and Stegun 1964, Percus 1971). For completeness, however, we outline a very simple, although quite crude estimate for c_N which is in remarkably good agreement with the asymptotic behaviour of the number of partitions of N for $N\to\infty$ (Abramowitz and Stegun 1964).

Consider only the vertical segments of the walk, and write N for N_{vert} in what follows. We must have

$$n_1<n_2<\ldots<n_k \tag{1}$$

with $\Sigma_{i=1}^{k} n_i=N$ and $1\leqslant k\leqslant k_{\max}$, with $k_{\max}$, the maximum number of segments in an N-step spiral, determined by the condition $\Sigma_{i=1}^{k_{\max}} i=N$. The latter constraint, corresponding to the 'tightest' possible spiral in which the length of each successive segment increases by 1, leads to $k_{\max}\sim\sqrt{2N}$. (We ignore the fact that the length of the last segment, n_k, may be arbitrary.) This gives

$$\begin{aligned} c_N &= \text{number of unequal partitionings of } N \\ &= \sum_{k=1}^{k_{\max}} \text{number of partitions of } N \text{ into } n_1<n_2<\ldots<n_k \\ &= \sum_k \frac{1}{k!}\,\text{number of partitions of } N \text{ into } k \text{ unequal groups.} \end{aligned} \tag{2}$$

We now relax the constraint $n_1<n_2<\ldots$ to $n_1\leqslant n_2\leqslant\ldots$. This corresponds to a spiral which has the possibility of occasionally tracing over its path as it expands. Thus our estimate for c_N will be an upper bound. We have

$$\begin{aligned} c_N &\simeq \sum_k \frac{1}{k!}\,\text{number of partitions of } N \text{ into } k \text{ groups of arbitrary sizes} \\ &= \sum_k \frac{1}{k!}\binom{N-1}{k-1}. \end{aligned} \tag{3}$$

At this stage, we write the sum as an integral and use Stirling's approximation to write the integrand in the form $\exp[f(k)]$. This gives

$$c_N\sim\frac{\sqrt{N}N^N}{2\pi}\int_0^{\sqrt{2N}}\exp[f(k)]\,\mathrm{d}k \tag{4}$$

with $f(k)=k-(N-k+\frac{1}{2})\ln(N-k)-(2k+1)\ln k$. We then perform this integral by writing $f(k)\simeq f(k_0)+\frac{1}{2}(k_0-k)^2f''(k_0)$, where k_0 is the value of k which maximises $f(k)$, and then evaluating the Gaussian integral. By setting $f'(k_0)=0$, we find $k_0\sim\sqrt{N}$, and by examining $f''(k_0)$, we find that the width of the peak of the distribution grows as $N^{1/4}$. Hence the customary next step of extending the upper limit of the resulting Gaussian integral to infinity is not entirely justified. Proceeding nevertheless, one obtains after performing a simple integral,

$$c_N\sim \mathrm{e}^{2\sqrt{N}}/(2\pi^{1/2}N^{1/4}). \tag{5a}$$

With this asymptotic form, one may easily derive that the generating function displays the following essential singularity near the critical point

$$G(x=1-\varepsilon)\simeq e^{1/4\varepsilon}. \tag{5b}$$

Our result in equation (5a) is of the same general form as the following asymptotic expression for the number of unequal partitions of the integer N quoted in Abramowitz and Stegun (1964)

$$c_N \simeq e^{\sqrt{N/3}}/(4\cdot 3^{1/4}N^{3/4}). \tag{6a}$$

In addition, the exact generating function for the partitioning problem is

$$G(x)=\prod_{N=1}^{\infty}(1+x^N) \tag{6b}$$

which can be readily shown to have an essential singularity as $x\to 1^-$ by taking the logarithm, expanding the multiple factors for x small, and then re-exponentiating the resulting expression.

To investigate the N-dependence of the exact c_N, we performed the following simple analysis. If c_N grows as ρ^{N^α}, then in terms of the successive ratios $r_N\equiv c_N/c_{N-1}$, the quantity $s_N=N^{1-\alpha}\log r_N$ should approach the constant $\alpha\log\rho$. A plot of s_N against $1/N$ for 3 values of α are shown in figure 3. Evidently, for the choice $\alpha=0.55$, the s_N do approach a constant which is approximately equal to 1.318, yielding the estimate $\rho\simeq 10.98$. This indicates that finite walks which are trapped in vortices represent a substantial contribution to the total number of walks, and this feature apparently shifts the growth law of the c_N from $\rho^{\sqrt{N}}$, predicted in equation (5a), to $\rho^{N^{0.55}}$. It should be noted from figure 1, however, that a terminating walk can be decomposed into two counter-rotating spirals. For each spiral, we expect the growth law of $\rho^{\sqrt{N}}$ should hold, so that the number of all walks should also grow at this rate. This last statement would be valid if the dominant contribution to all walks came from superposing two counter-rotating spirals with approximately equal number of steps. Thus our conclusion that c_N does grow more rapidly than $\rho^{\sqrt{N}}$ may be due to the extremely slow convergence of the series.

While c_N has a novel N-dependence, $\langle R_N^2\rangle$ and $\langle\theta_N\rangle$ do appear to diverge as simple power laws in N. Defining exponents by $\langle R_N^2\rangle\sim N^{2\nu}$ and $\langle\theta_N\rangle\sim N^{\nu_\theta}$, we find that the

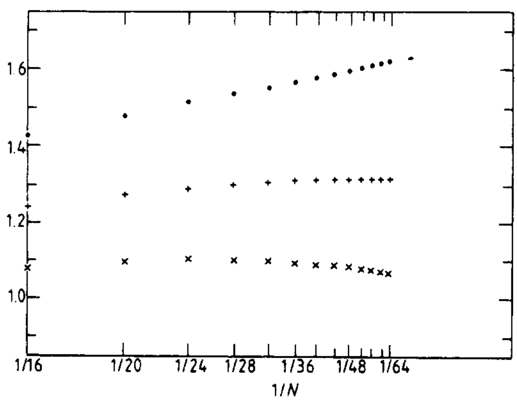

Figure 3. A plot of $s_N=N^{1-\alpha}\log(c_N/c_{N-1})$ against $1/N$ for three choices of α: $\alpha=0.50$ (●), $\alpha=0.55$ (+), and $\alpha=0.60$ (×).

ratio extrapolants for ν are strongly N-dependent. However, by order 65 a clear trend is reached which suggests that $\nu \simeq 0.60$. Ratio extrapolants for ν_θ are much better behaved than those for ν, and we estimate $\nu_\theta \simeq 0.55$. This exponent value explains why the c_N apparently vary as $\rho^{N^{0.55}}$, rather than as $\rho^{\sqrt{N}}$. The mean rotation angle should be approximately equal to one-fourth the total number of segments in the spiral. From our analysis leading to equation (5), we saw that the typical number of segments in the spiral, k_0, (as well as the expected length of the longest segment in the spiral) should both increase as $\sqrt{N}$. This $\sqrt{N}$ behaviour immediately gives a $\rho^{\sqrt{N}}$ dependence of the c_N. If, however, the typical number of segments increases as $N^{0.55}$, then c_N should vary as $\rho^{N^{0.55}}$. The former alternative is suggested by the analytical approach, while the latter is suggested by our series data.

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