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LETTER TO THE EDITOR

Spiralling self-avoiding walks: an exact solution

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Abstract. An exact solution is presented to a problem of spiralling self-avoiding walks on the square lattice recently proposed by Privman. For $N \to \infty$, the number of N-step spiral walks increases as $c_N \simeq 2^{-2}3^{-5/4}\pi N^{-7/4} \exp[2\pi(N/3)^{1/2}]$, and their root-mean-square end-to-end distance behaves as $R_N \simeq \frac{1}{2}\sqrt{3}\pi^{-1}N^{1/2} \log N$.

In a recent letter Privman (1983) considers a new and interesting self-avoiding walk (SAW) problem. For this problem, defined on the square lattice, the bond angles are subject to a constraint: when the SAW is traversed in a given sense, then each bond may either point in the same direction as the preceeding one, or in a direction rotated by $+\pi/2$ with respect to it. The global behaviour that results from the combination of two local constraints (the excluded volume and the bond angle restrictions) is quite striking: in general a SAW obeying these constraints consists of an outward spiralling part and an inward spiralling part (figure 1). The question then arises to which universality class these spiralling SAWs belong.

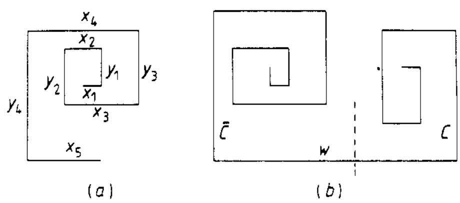

Figure 1. (*a*) An outward spiralling SAW. The segment lengths are indicated. (*b*) In general, a spiralling SAW consists of an outward spiralling part $\bar{C}$ and an inward spiralling part C. The dividing line (broken) intersects the dividing segment w.

We shall let c_N denote the total number of N-step walks and R_N their root-mean-square end-to-end distance. By enumeration Privman (1983) obtained c_N and R_N for $N \leq 40$. Upon assuming that asymptotically

$$c_N \sim \mu^N N^{\gamma-1}, \qquad R_N \sim N^\nu \tag{1}$$

(as for ordinary SAWs) this author estimated with the aid of series analysis techniques that

$$\mu = 1.15 \pm 0.15, \qquad \gamma = 5.2 \pm 1.3, \qquad \nu = 0.62 \pm 0.06. \tag{2}$$

The estimates of the exponents γ and ν are well away from the usual two-dimensional SAW values $\gamma = \frac{43}{32}$ and $\nu = \frac{3}{4}$ (Nienhuis 1982, 1984). However, the error margins are quite large for a series of this length. We have independently reproduced Privman's numbers and extended the series to 50 terms (table 1). Subsequent ratio analysis suggests that ν may be less than 0.62, but the accuracy remains unsatisfactory. These circumstances have led us to attack the problem by analytical means.

Table 1. Numerical data for spiral SAWs for $40 < N \leq 50$: the number c_N of N-step walks, and the sum of the squared end-to-end distances $c_N R_N^2$.

N	c_N	$c_N R_N^2$	N	c_N	$c_N R_N^2$
41	2 444 270	191 568 966	46	8 106 019	733 331 452
42	3 121 064	252 134 740	47	10 232 851	950 690 811
43	3 977 420	330 781 244	48	12 885 792	1 229 086 888
44	5 053 839	432 606 792	49	16 196 772	1 584 784 532
45	6 409 117	564 069 533	50	20 312 050	2 038 147 096

Here we present an exact solution to the problem posed by Privman. We first solve the easier problem of the subclass of SAWs that only spiral outward (figure 1(a)). For the quantities c'_N and R'_N referring to this subclass we find that for $N \to \infty$

$$c'_N \simeq \tfrac{1}{4}\sqrt{2}\pi^{-1}N^{-1/2}\kappa^{\sqrt{N}}, \tag{3}$$

$$R'_N \simeq \tfrac{1}{2}\sqrt{3}\pi^{-1}N^{1/2}\log N. \tag{4}$$

Here

$$\kappa = \exp(\pi\sqrt{\tfrac{2}{3}}) = 13.00195 \tag{5}$$

is the same constant that appears in the famous problem of the number of partitions of an integer N, solved in a celebrated paper by Hardy and Ramanujan (1918) (see also Andrews (1976)). It also occurs in a specific lattice animal problem (Derrida 1983).

Upon extending our solution to the full problem of all spiralling SAWs we obtain

$$c_N \simeq 2^{-2}3^{-5/4}\pi N^{-7/4}\kappa^{\sqrt{2N}}, \tag{6}$$

$$R_N \simeq \tfrac{1}{2}\sqrt{3}\pi^{-1}N^{1/2}\log N. \tag{7}$$

The functional form of c_N is clearly different from the one assumed in (1). The behaviour of R_N is described by an exponent $\nu = \frac{1}{2}$ and a logarithmic correction factor. We shall first expose our method of solution, then comment on the differences between (5)–(7) and (1)–(2), and finally discuss why numerical analysis is unable to give accurate results even with a series as long as 50 terms.

Our approach is to calculate the generating function

$$G(z) = \sum_{N=1}^{\infty} c_N z^N \tag{8}$$

for the full problem and the analogous quantity $G'(z)$ for the subclass of outward spiralling SAWs. These are just the partition functions of grand ensembles characterised by a step fugacity z. We begin by studying $G'(z)$ (see figure 1(a)). A spiral can be decomposed into x and y segments, parallel to the x and y axes, respectively. We adopt the convention that each spiral has its last (i.e. outermost) segment parallel to the x axis. We denote the segment lengths by the integers $x_1, x_2, \ldots, x_{L+1}$ and $y_1, y_2, \ldots, y_L$, as defined in figure 1(a). The above convention implies that $0 \leqslant x_1 < x_2 < \ldots < x_L$, $x_{L+1} \geqslant 1$, and $1 \leqslant y_1 < y_2 < \ldots < y_L$ (the case $x_1 = 0$ corresponding to a walk that leaves its origin in the y direction). The generating function $G'(z)$ is obtained as a sum over the segment lengths and over the number of segments,

$$G'(z) = \sum_{L=0}^{\infty} \sum_{0 \leqslant x_1 < \ldots < x_L} \sum_{1 \leqslant x_{L+1}} \sum_{1 \leqslant y_1 < \ldots < y_L} z^{x_1 + \ldots + x_{L+1} + y_1 + \ldots + y_L}. \tag{9}$$

The sum over x_{L+1} can be carried out directly, and the remaining sums (which are absent if $L = 0$) can all be decoupled by transformation to $m_1 = x_1$, $n_1 = y_1$ and $m_k = x_k - x_{k-1}$, $n_k = y_k - y_{k-1}$ ($k = 1, 2, \ldots, L$). As a result we obtain for the generating function of the subclass of outward spiralling SAWS

$$G'(z) = \frac{z}{1-z} \sum_{L=1}^{\infty} g_{L-1}(z)[g_{L-1}(z) + g_L(z)] \tag{10}$$

where $g_0(z) \equiv 1$ and

$$g_L(z) = \prod_{l=1}^{L} \frac{z^l}{1-z^l}, \qquad L = 1, 2, \ldots . \tag{11}$$

It is easy to show that the series in (10) has 1 as its radius of convergence. Our task then is to relate the $z \to 1$ behaviour of $G'(z)$ to the large N behaviour of c'_N. We shall indicate only the principal steps of the calculation. First of all one notices that at fixed z the quantity $g_L(z)$ takes its maximum value for $L = L_0(z)$ where $L_0(z)$ is the integer part of $\log \frac{1}{2} / \log z$. For $z = 1 - \varepsilon$ and $\varepsilon \to 0$ the main contribution to the sum in (10) is expected to come from values $L \approx L_0 \approx (\log 2)/\varepsilon$. Also, in this limit the two terms in brackets will contribute equally. As $\varepsilon \to 0$ we therefore have to leading order

$$G'(z) \simeq \frac{2}{\varepsilon} \exp\left(-2 \sum_{m=1}^{L_0} \log(z^{-m} - 1)\right) \sum_{L=1}^{\infty} \exp\left(2 \sum_{l=L_0+1}^{L} \log(z^{-l} - 1)\right) \tag{12}$$

where $\Sigma_{l=L_0+1}^{L}$ stands for $-\Sigma_{l=L+1}^{L_0}$ if $L < L_0$. For small ε the quantity $\log(z^{-l} - 1)$ varies only slowly near $l = L_0$. Hence the sums over l and L in (12) may be replaced by integrals, and the integral over L can be calculated, to leading order in ε, by the steepest-descent method. This contributes a factor $(\pi/2\varepsilon)^{1/2}$. Furthermore, the sum in the prefactor in (12) is found to behave asymptotically as $-\pi^2/(12\varepsilon) + \frac{1}{2}\log(2\pi/\varepsilon) + o(1)$. Putting these results together we find, for $z = 1 - \varepsilon$ and $\varepsilon \to 0$,

$$G'(z) \simeq (2\pi\varepsilon)^{-1/2} \exp(\pi^2/6\varepsilon). \tag{13}$$

Next, asymptotic evaluation of the Laplace inverse

$$c'_N = (2\pi \mathrm{i})^{-1} \oint (G'(z)/z^{N+1})\, \mathrm{d}z \tag{14}$$

for large N yields (3). It is now easy to obtain from (13) the average chain length $N'(z)$ in the ensemble described by $G'(z)$. For $\varepsilon \to 0$ we have

$$N'(z) = \mathrm{d} \log G'(z) / \mathrm{d} \log z \simeq \pi^2/6\varepsilon^2. \tag{15}$$

A second differentiation shows that the root-mean-square fluctuations $\Delta N'(z)$ satisfy

$\Delta N'/N' \sim (N')^{-1/4}$, i.e. the relative fluctuations are larger than in a usual statistical problem, but still vanish as $N' \to \infty$.

The calculation of the root-mean-square end-to-end distance $R'(z)$ in the grand ensemble poses no problem of principle. The starting point is the expression for the squared end-to-end distance r_L^2 of a chain with a number L and y segments and a number $L+1$ (or L, if $x_1 = 0$) of x segments,

$$r_L^2 = \left(\sum_{l=1}^{L+1} (-1)^l x_l\right)^2 + \left(\sum_{l=1}^{L} (-1)^l y_l\right)^2. \tag{16}$$

Once this expression has been inserted inside the summations of (9), the calculation of its average $R'(z)$ is straightforward. It requires the asymptotic evaluation of several sums. We give the result for $z = 1-\varepsilon$ with $\varepsilon \to 0$,

$$R'(z) \simeq (2/\varepsilon^2)[(\tfrac{1}{2}\log(2/\varepsilon))^2 - \tfrac{1}{2}(1-\gamma)\log(2/\varepsilon) + 1 - \tfrac{1}{2}\gamma + \tfrac{1}{4}\gamma^2 + \tfrac{1}{8}\pi^2] \tag{17}$$

where $\gamma = 0.57722$ is Euler's constant. Correction terms to (17) are smaller than the leading ones by at least a factor ε, apart from logarithms. Equation (4) follows by combining (15) and (17).

We consider now the full problem of all spiralling SAWs (see figure 1(b)). In order to write down their generating function $G(z)$ we introduce the concept of a *dividing line.* By this we shall mean a line parallel to the x or the y axis which intersects only a single segment of the walk. This segment will be called the *dividing segment.* One easily sees the following properties.

(i) Each spiralling SAW (of the general type figure 1(b)) has either one or two dividing lines.

(ii) In the latter case the dividing segments are neighbouring segments.

(iii) If a dividing segment is deleted, the result is two disjunct spirals to be called C and $\bar{C}$. The spirals C or $\bar{C}$ may be 'empty'. For SAWs with two dividing segments two such decompositions are possible.

The generating function $G(z)$ is most easily calculated if one writes down summations over the configurations C and $\bar{C}$ separately, and inside this double summation a sum over all allowed lengths w of the dividing segment connecting C and $\bar{C}$; w has a minimum value determined only by the outer segments of C and $\bar{C}$. In this way, however, SAWs with two dividing segments are counted twice, and one must subtract a correction term. This term consists again of a double summation, say over C' and $\bar{C}'$, but now with an inner sum over the length of *two* dividing segments. In both the main term and the correction term the sums over the dividing segment(s) can be carried out and result in a decoupling of the remaining sums over the inward and outward spirals. We skip intermediate results and present our final expression for $G(z)$,

$$G(z) = [z/(1-z)] + 2\Omega(z) + [(1-z)(2z-1)/z^2]\Omega^2(z) \tag{18}$$

where the function $\Omega(z)$ is defined as

$$\Omega(z) = \sum_{L=1}^{\infty} g_L(z)[g_L(z) + g_{L+1}(z)] \tag{19}$$

and related to the partition function $G'(z)$ by

$$\Omega(z) = [(1-z)/z][G'(z) - z/(1-z)^2]. \tag{20}$$

We have checked that Taylor expansion of (18) correctly reproduces c_1–c_{10}. From (18) and (20) we see that for $z=1-\varepsilon$ and $\varepsilon\to 0$

$$G(z)\simeq\varepsilon^3(G'(z))^2. \tag{21}$$

This shows the $G(z)$ also becomes singular at $z=1$, and hence we have $\mu=1$ for this problem. Equation (21), together with the result (13) for $G'(z)$ and after Laplace inversion, yields (6) for c_N. In analogy to (15)

$$N(z)\simeq\pi^2/3\varepsilon. \tag{22}$$

Finally, we have calculated the root-mean-square end-to-end distance in the full ensemble of spiralling SAWs. The result is, for $z=1-\varepsilon$ and $\varepsilon\to 0$,

$$R(z)\simeq(4/\varepsilon^2)[(\tfrac{1}{2}\log(2/\varepsilon))^2-\tfrac{1}{2}(1-\gamma)\log(2/\varepsilon)-\tfrac{1}{2}\gamma+\tfrac{1}{4}\gamma^2+\tfrac{1}{8}\pi^2]. \tag{23}$$

From (22) and (23) one obtains, to leading order, equation (7).

Several comments are in place. First of all, the increase of c_N and c'_N as exponentials of $N^{1/2}$ (equations (3) and (6)) rather than of N (equation (1)) becomes clear if one realises that the only effective degrees of freedom of a spiralling SAW are its turning points, of which there are $\sim N^{1/2}$. This may explain the difficulty of analysing even a series of 50 terms. We found that the coefficients c_N for $1\leqslant N\leqslant 40$ are fitted better by Privman's formulae, (1) and (2), than by our exact asymptotic expression, (5) and (6)!

A supplementary difficulty in analysing the series for R_N is caused by the logarithms in (17). If one defines an effective exponent as a function of N by $\nu_N=\mathrm{d}\log R_N/\mathrm{d}\log N$, then this factor contributes an extremely slowly vanishing correction to the asymptotic value $\nu=\frac{1}{2}$:

$$\nu_N=\tfrac{1}{2}+1/\log N+\mathrm{O}(1/\log^2 N). \tag{24}$$

This shows clearly why performing a series analysis without any knowledge about the functional forms of c_N and of R_N did not give satisfactory results.

Finally we remark that for this system not only the mean-square end-to-end distance but also all other pair and higher-order correlation functions can be calculated. We conclude that we are dealing with an exactly solvable yet non-trivial excluded volume problem.

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References

Andrews G E 1976 *The Theory of Partitions* (London: Addision-Wesley)
Derrida B 1983 *Private communication*
Hardy G H and Ramanujan S 1918 *Proc. London Math. Soc.* (2) **17** 75
Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
—— 1984 *J. Stat. Phys.* **34**
Privman V 1983 *J. Phys. A: Math. Gen.* **16** L571