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1984 J. Phys. A: Math. Gen. 17 L271

(http://iopscience.iop.org/0305-4470/17/5/010)

J. Phys. A: Math. Gen. 17 (1984) L271–L274. Printed in Great Britain

LETTER TO THE EDITOR

On the number of spiral self-avoiding walks

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Received 11 January 1984

Abstract. We consider the problem of spiral self-avoiding walks as recently introduced by Privman. We prove that the number of n-step spiral self-avoiding walks is given by

$$s_n = \exp[2\pi(n/3)^{1/2}]/(n^{7/4}c)[1+O(1/\sqrt{n})]$$

where $c = \pi/(4.3^{5/4})$. Similar results for various subsets of these walks are also obtained.

Very recently Privman (1983) introduced the problem of 'spiral' self-avoiding walks (SSAW's) on the square lattice. These walks possess, in addition to the usual self-avoiding constraint, the property that left-hand turns are forbidden. As a consequence, SSAW's may only expand linearly or spiral outwards. Failure to do either results in the walk being trapped, and unable to grow.

Privmann enumerated the SSAW's with up to 40 steps (s_n; $n=1$, 40), and their mean square end-to-end distance (ρ_n; $n=1, 40$), and, on the basis of a conventional series analysis, suggested that $s_n \sim \mu^n n^{\gamma-1}$ and $\rho_n \sim c \cdot n^{2\nu}$ where $\mu = 1.15 \pm 0.15$, $\gamma = 5.2 \pm 1.3$ and $\nu = 0.62 \pm 0.06$, in analogy with the behaviour of normal self-avoiding walks, for which similar functional forms apply, but with different values for μ, γ and ν.

Subsequently, Redner and De Arcangelis (1984) extended the series to 65 terms, and pointed out that the spiral constraint imposes upon the walks a characteristic behaviour similar to the number of partitions of the integers into distinct parts. As this quantity is known to grow like $\rho^{\sqrt{n}}$, they reanalysed the walk generating function for a growth function of this form and concluded that the series were suggestive of $s_n \sim \rho^{n^\alpha}$ with $\alpha \approx 0.55$. This exponent estimate derived from a ratio analysis in which $n^{\alpha-1}\log(s_n/s_{n-1})$ was extrapolated against $1/n$. However, it is clear that if $\alpha = \frac{1}{2}$, the extrapolants will behave like $k_0[1+k_1/\sqrt{n}+O(1/n)]$. Thus extrapolation against $1/n$ will not be linear, due to the curvature induced by the $O(1/\sqrt{n})$ term. It is this factor that caused Redner and De Arcangelis to estimate $\alpha \approx 0.55$, (rather than the correct value $\alpha = \frac{1}{2}$) which has the (local) effect of reducing the curvature in the ratio plots.

Privman's form also fits the data quite well locally, certainly better than the asymptotic form we obtain, which is still some 30% in error at $n = 65$. The slow convergence is partly due to the correction term being $O(1/\sqrt{n})$ rather than $O(1/n)$ as is the case with more conventional forms of series.

In the next section we show that the correct asymptotic form can be derived by considering the number of partitions of the integer n into k distinct parts, $q(n, k)$.

0305-4470/84/050271+04$02.25

The fundamental result needed is due to Szekeres (1951) and is

$$q(n, k) \sim \{a \log 2/2\pi n[2(a-1)]^{1/2}\} \exp[\pi(n/3)^{1/2}(1-F\lambda^2)] \qquad (1)$$

where $a = \frac{1}{12}(\pi/\log 2)^2$, $F = (a-1)/2a^2$ and

$$k+\tfrac{1}{2} = (n+\tfrac{1}{16})^{1/2}a^{-1/2}[1+(1-1/a)\lambda + \text{constant } \lambda^2 + O(\lambda^3)] \qquad (2)$$

where $\lambda = O(n^{-1/2})$. Note that $k = O(\sqrt{n})$. Szekeres also showed that $q(n, k)$ is monotonic in k for n large, except at the peak (where $k \sim (n/a)^{1/2}$).

We specify the first step of the walk to be vertically upwards. All SSAW's exist as either a single 'spiral' (figure 1(a)) or a double spiral (figure 1(b), (c)). Note that the purely linear walk, or walks with only one turning point, are just simple cases of single spirals. Each SSAW can be decomposed into a concatenation of two walks of a particular type by either a vertical line (figure 1(a) and (b)), a horizontal line (1(c)) or in some cases both (1(d)). The cutting line chosen is the appropriate line such that the last linear segment of the spiral OA is equal to the length of the third last segment (the relevant segments are shown bold in figure 1). In 1(d) the vertical cutting line shown is the appropriate line for the reversed walk.

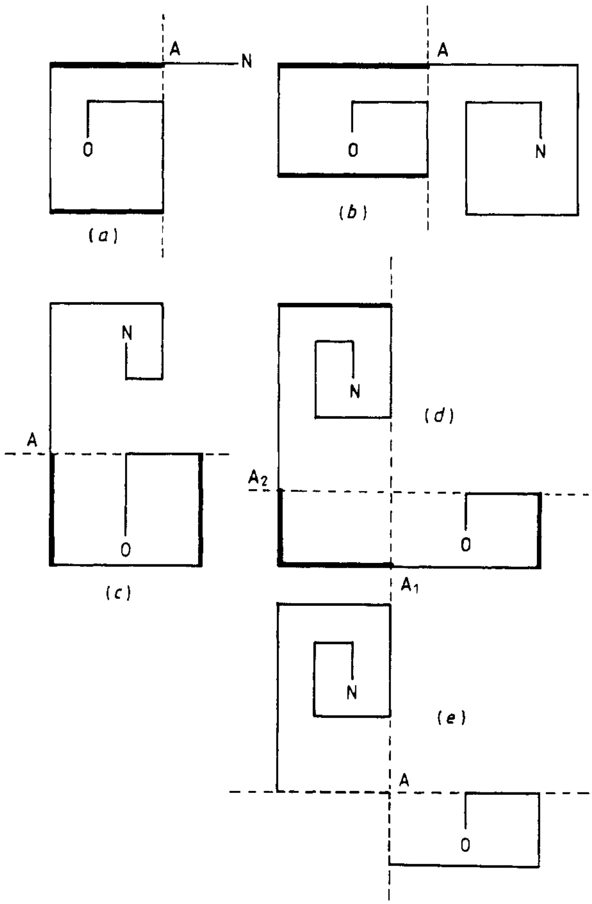

Figure 1. A variety of spiral self-avoiding walks with origin O and end-point N. The cutting line (see text) is shown broken.

Let S_n denote the set of n-step SSAW's with cardinality s_n. Let I_n denote the set of n-step SSAW's discussed above; that is, SSAW's whose last and third last segments are of equal length. Let C_n denote a class of spiral walk whose last segment is at least one greater than the length of the third last segment. Finally, we denote the set of 'live' walks by L_n, and these are defined to be single spirals (isomorphic to 1(a)) with the second last segment greater than the fourth last segment. Such walks can always be continued indefinitely, hence the name. Denote the cardinalities of I_n, C_n and L_n by i_n, c_n and l_n respectively. From figure 1(a)–1(d), it is clear that the section of the spiral from O to A belongs to I_k, while that from A to N belongs to C_{n-k}, and the walks 1(a), (b) and (c) can be uniquely decomposed in this way. Thus we can write

$$s_n = \sum_{k\geqslant 0} i_k c_{n-k} - \sum_{k\geqslant 0} i_k i_{n-k}. \tag{3}$$

The second sum corrects for walks of type d, which will be counted twice by the first sum. Figure 1(e) shows the geometrical construction that uniquely transforms such walks (as in 1(d)) into two concatenated walks from the set I. Note too that detailed definitional specifications such as i_0 are needed for (3) to be universally applicable. We have shown that these cases do not contribute to leading order, and so prefer to neglect them at this stage. Equation (3) can be used, together with (4) and (5) for efficient calculation of the numbers s_n. Next, if one considers the possible ways to 'grow' a member of class C_{n+1}, it can be seen that such walks are obtainable by adding a step in a particular direction to each member of $C_n \cup I_n$. Thus

$$c_{n+1} = c_n + i_n. \tag{4}$$

Now the length of the vertical and horizontal segments of C_n must independently satisfy $n_1 < n_2 \ldots < n_m$ where n_i numbers the length of the ith linear segment counting from the origin. Let the total number of vertical (horizontal) steps be $n_V(n_H)$, so that $n_V + n_H = n$. Further, if the number of horizontal segments is k, the number of vertical segments is either k or $k+1$ (figure 1(b) and (c)). Thus

$$c_n = \sum_{k=1}^{n} \sum_{j=1}^{n} q(j,k)[q(n-j,k) + q(n-j,k+1)] \tag{5}$$

where $q(j,k)$ is defined in (1). Now (1) implies that (5) is at least of the order of $[\tilde{q}(n/2)]^2/n^4$ where $\tilde{q}(n)$ is the number of partitions of n into distinct parts. It follows that we need only consider terms with $j = \frac{1}{2}n + O(n^{0.8})$. Using (1) and estimating the sums by integrals, a considerable amount of algebra then yields

$$c_n = (1/4\sqrt{3n}) \exp[\pi(2n/3)^{1/2}][1 + (c/\sqrt{n}) + O(1/n)] \tag{6}$$

for some constant c. The form of the correction terms here follows easily from the method of Szekeres. From (4) we then obtain

$$i_n = (\pi/12\sqrt{2}3^{3/2}) \exp[\pi(2n/3)^{1/2}][1 + O(1/\sqrt{n})]. \tag{7}$$

Further, as a by-product of this analysis we find for live spirals

$$l_n = (1/2\sqrt{2}\pi\sqrt{n}) \exp[\pi(2n/3)^{1/2}][1 + O(1/\sqrt{n})]. \tag{8}$$

Substituting (6) and (7) into (3) we see that the largest terms in the sum are those in the vicinity of $k = n/2$. Expanding around this maximum, and again replacing the sum by an integral, we finally obtain

$$s_n = (\pi/4.3^{5/4}.n^{7/4}) \exp[2\pi(n/3)^{1/2}][1+O(1/\sqrt{n})] \tag{9}$$

where we have neglected the second sum in (3), it being $O(1/n)$ compared to the first. The form of the correction term in (9) $[O(1/\sqrt{n})]$ is obtained by retaining the necessary correction terms at all stages, including the proofs in Szekeres (1951).

We have found the asymptotic form for the number of n-step spiral self-avoiding walks embeddable in the square lattice. A crude numerical calculation gives the correction term to (9) as $\beta/\sqrt{n}$, with $\beta \approx -0.7$. Similar asymptotic forms for related subsets of spiral walks are also obtained.

After the completion of this work we became aware of calculations of Blöte and Hilhorst (1984) and of Klein *et al* (1984). Blöte and Hilhorst obtain the same results as ours, though by a completely different method and without any error bounds. They also obtain the asymptotic form for the mean square end-to-end distance. Klein *et al* incorrectly obtain $s_n \sim n^{-5/4} \exp[2\pi(n/3)^{1/2}]$, though they correctly find $c_n \sim n^{-1} \exp[\pi(2n/3)^{1/2}]$.

These calculations certainly confirm that SSAW's belong to a different universality class than ordinary SSAW's. It seems however, that they are more of combinatorial significance than of statistical mechanical significance.

We are most grateful to Professor George Szekeres for his comments on, and corrections to, the manuscript.

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