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LETTER TO THE EDITOR

Spiralling self-avoiding walks†

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Abstract. Self-avoiding walks which only step straight-ahead or to the left are studied. Heuristic arguments, generating function studies, and extrapolation of few-step enumerations are described. Exact asymptotic results are obtained. It is found that these spiralling walks are in a new 'universality class', wherein the number of n-step walks does not behave in a 'size-extensive' manner.

The incorporation of volume exclusion when embedding structures on a lattice seems to be a difficult problem with many applications. For instance, self-avoiding walks (SAWs) have received wide attention as simple models for chain polymers (see, e.g., deGennes 1979). The functional form for the asymptotic behaviour of various properties as a function of walk length identifies a general 'universality class', and it is of interest to determine what modifications change this classification. SAWs with a different weight for stepping straight ahead but equal (non-negative finite) weights for any turn, evidently belong to the same universality class, whereas SAWs with a weight anisotropically directed with reference to a fixed lattice direction are in another class (see, e.g., Nadal *et al* 1982, or Redner and Majid 1983). Recently Privman (1983) has suggested that SAWs with a preference for turning counterclockwise might be in yet another universality class.

Here on the square-planar lattice we study such SAWs turning only in one direction as one proceeds along the walk from one end to the other. Typically these walks have a scroll-like structure such as illustrated in figure 1. But these scroll-like walks can be separated, as indicated by the arrow in figure 1, into two purely spiralling SAWs which should exhibit much the same asymptotic behaviour. The number c_n and the root-mean-square end-to-end separation r_n of such n-step purely spiralling SAWs are expected to exhibit asymptotic behaviour

$$c_n \sim n^{\alpha} \exp(an^{\mu}) \tag{1}$$

$$r_n \sim n^{\nu}. \tag{2}$$

Should it turn out that $\mu \neq 1$, then the conformational entropy $\ln c_n$ would not be 'size-extensive' (in terms of n as a measure of size).

Heuristic arguments involving the exponents μ and ν can be made. Consider the process of 'growing' outward spiralling SAWs: each step is taken either to the left or

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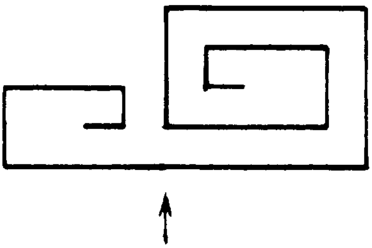

Figure 1. An example of a SAW turning only counterclockwise as one proceeds along the walk from the left end.

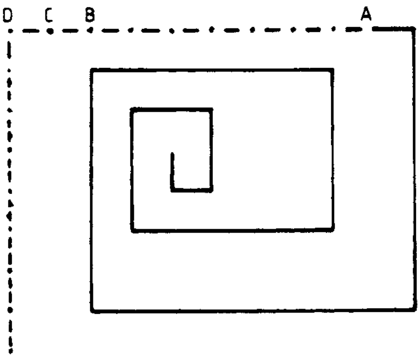

Figure 2. An example of a purely spiralling SAW.

straight ahead with equal probability; if any preceding portion of the walk is encountered the growth process fails and is re-initiated for another walk†. Now while proceding along a side as from A to B in figure 2, any (left) turn will (at least, eventually) lead to failure; but following B along to C there are two choices which do not lead to (eventual) certain failure; once a turn is made, say at D, there is again a period along a side with only one choice avoiding certain failure; etc. Since the average length of a side should be $\sim r_n \sim n^{\nu}$ and since the average number of steps beyond a side (as from B to D in figure 2) might be expected to be finite (say $1 < \Delta \sim n^0$), the average fraction of times that a non-unique failure-avoiding choice is possible is $\simeq \Delta/(n^{\nu}+\Delta) \simeq \Delta/n^{\nu}$. Since it is only with these non-unique failure-avoiding choices that there are non-identity (multiplicative) contributions to c_n, we anticipate that $c_n \sim k^{n(\Delta/n^{\nu})} = k^{\Delta(n^{1-\nu})}$. Thus a relation between exponents appearing in equations (1) and (2) is indicated,

$$\mu + \nu = 1. \qquad (3)$$

Next let m_n denote the average number of turns in a spiral and note that the average distance between the ith and $(i+1)$th turns should be $\sim i\Delta$. Then we anticipate that

$$n \sim \sum_{i=1}^{m_n} i\Delta \sim m_n^2 \Delta \quad \text{or} \quad m_n \sim n^{1/2}. \qquad (4)$$

Moreover since the last side of an average spiral should have a length $\sim m_n\Delta$, the spiral size r_n should scale $\sim m_n\Delta$, so that

$$\mu = \tfrac{1}{2} \quad \text{and} \quad \nu = \tfrac{1}{2} \qquad (5)$$

(where equation (3) has been recalled).

Further arguments can be made based upon a particular labelling of the outward spiralling SAWs, which we shall restrict so that its last vertical side is longer than previous successive progressions of vertical steps, and similarly for the horizontal case.

† In treating SAWs it is generally of crucial importance to account either explicitly (as summarised in Wall 1964, or Windwer 1970) or implicitly (via 'weights', as summarised in Windwer 1970, or McCrackin 1972) for such 'failures' and 're-initiations' so as to obtain the desired statistics where each possible SAW is counted equally.

Then the progressions of successive vertical steps (strictly) increase as one cycles outward from the centre of a cycle. Thus if there are v vertical steps each possible sequence of vertical progressions is uniquely identified by the *partition* of v whose *parts* are the lengths of these progressions. A similar partition of h, the number of horizontal steps, uniquely identifies the horizontal progressions, the number of which can differ by no more than one from the number of vertical progressions. Clearly, then there is essentially† a one-to-one correspondence between our spirals and a pair of such partitions, each restricted to have distinct parts the number of which differ by no more than one in each partition. Thus the spiralling walk problem is framed in terms of partitions, the theory of which is extensive (e.g., in Hardy and Wright 1938, or Andrews 1976).

We consider the class $\mathscr{C}(j, m)$ of partitions of j such that there are m unequal parts (≥ 1) in each partition. Now the members of $\mathscr{C}(j, m)$ are in one-to-one correspondence with the members of the class $\tilde{\mathscr{C}}(j, m)$ of partitions of j such that the only parts are $1, 2, \ldots, m$ each occurring at least once. This result may be seen on representing partitions in terms of a Young diagram (or Ferrer's graph), such as illustrated in figure 3. The correspondence between the members of $\mathscr{C}(j, m)$ and $\tilde{\mathscr{C}}(j, m)$ is simply that between the diagram of the partition and that with the *conjugate* diagram, obtained by rotating a diagram (by π) about the diagonal axis passing through the upper left-hand corner. (For instance, the two diagrams in figure 3 are conjugate.) Thus the classes $\mathscr{C}(j, m)$ and $\tilde{\mathscr{C}}(j, m)$ have the same order $|\mathscr{C}(j, m)| = |\tilde{\mathscr{C}}(j, m)|$. Further they have the same generating function

$$f_m(t) \equiv \sum_{j\geq 1} |\mathscr{C}(j, m)| t^j = \sum_{j\geq 1} |\tilde{\mathscr{C}}(j, m)| t^j. \tag{6}$$

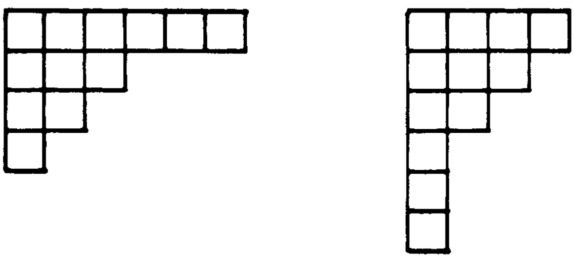

Figure 3. Two examples of Young diagrams corresponding to partitions of 12, namely [6, 3, 2, 1] and [4, 3, 2, 1, 1, 1].

Now via standard considerations (as in Hardy and Wright 1938) the generating function for $\tilde{\mathscr{C}}(j, m)$ is seen to be

$$f_m(t) = \prod_{i=1}^{m} t^i (1 - t^i)^{-1}. \tag{7}$$

Of course $|t| < 1$ so that $(1 - t^i)^{-1}$ can be expanded as $\Sigma_{j\geq 0} t^{ij}$. The desired generating function for spiralling SAWs is defined by

$$F(t) \equiv \sum_{n\geq 1} c_n t^n. \tag{8}$$

† Actually to achieve this we need also to fix the origin and the direction of the first step of the spirals.

Because of the correspondence of these SAWs with pairs of partitions (with m-values differing by no more than one), we have

$$F(t)=\sum_{m\geq 1} f_m(t)\{f_m(t)+2f_{m-1}(t)\}. \tag{9}$$

Now $F(t)$ may be used to study spiralling SAWs. First the (m)th and $(m-1)$th terms of (9) are compared, the ratio of the (m)th to $(m-1)$th terms being $t^{2^m}(1+t^{m+1})(1-t^{2^m})^{-1}(1-t^{m+1})^{-1}$ and we see that no matter how small $1-|t|>0$ is, there exists an m-value beyond which this ratio has a decreasing magnitude <1. Thus the series of (9) is convergent for $|t|<1$; and from (8) it is seen that for any $|t|<1$, the $|c_n t^n|\to 0$ as $n\to\infty$. Consequently it is established that $\mu<1$. Moreover, since as $t\to 1^-$ higher terms in (8) become more important, the asymptotic behaviour of $F(t)$ as $t\to 1^-$ can be used to deduce the asympotic behaviour of c_n as $n\to\infty$. To this end we seek the terms in (9) which make the dominant contributions. From (7) these contributions are seen to occur near the m-value

$$m_0\equiv(\ln 2)/\ln(t^{-1}) \tag{10}$$

where $f_m(t)$ is a maximum. Then expanding the logarithm of the summand in (9) about the maximum value at $m=m_0$, we find that, as $t\to 1^-$,

$$\ln F(t)\to\ln\left(3[f_m(t)]^2\sum_m \exp-[2(\ln t^{-1})(m-m_0)^2]\right)$$
$$\to 2\int_0^{\ln 2}\{x+\ln(1-e^{-x})\}\,\mathrm{d}x(\ln t^{-1})^{-1}+\tfrac{1}{2}\ln(\ln t^{-1})+(\text{constant}). \tag{11}$$

Next if a functional form as in (1) is assumed for c_n and substituted in (8), then for $t\to 1^-$ it may be shown that

$$\ln F(t)\to\frac{1-\mu}{\mu}(a\mu)^{1/(1-\mu)}(\ln t^{-1})^{-\mu/(1-\mu)}$$
$$-\frac{\alpha+1-\mu/2}{1-\mu}\ln(\ln t^{-1})+(\text{constant}). \tag{12}$$

Upon comparison of the expressions in (11) and (12) one sees that $\mu=\frac{1}{2}$ (in agreement with our expectation) and $\alpha=-1$. Numerical evaluation of the integral in (11) yields an estimate for $a\cong 2.565\,096\,60$. This value is very close to $\pi\sqrt{2/3}$, a constant which arises (see, e.g., Andrews 1976) in the enumeration of all partitions (of large integers).

Another generating function $G(t)$ may be introduced to check some other aspects of our heueristic argument. Let $G(t)$ be the generating function essentially for c_n times the average number m_n of turns in an n-step spiral; we define it as

$$G(t)\equiv\sum_{m\geq 1} mf_m(t)\{f_m(t)+2f_{m-1}(t)\} \tag{13}$$

Assuming again (1) and $m_n\sim n^{\beta}$, we find that an asymptotic analysis like that already described for $F(t)$ leads to $\beta=\frac{1}{2}$, in agreement with (4).

Next the relation between the class of purely spiralling SAWs and the more general class including scroll-like structures is addressed. Keeping in mind the process for joining a pair of pure spirals to form a scroll, as indicated in figure 1, we anticipate the number c'_n of n-step scroll-like SAWs to be related to counts for the pure spirals,

$$c'_n \sim \sum_{p=0}^{n} c_p c_{n-p}. \tag{14}$$

(The proportionality constant here should be the inverse of an average number of steps located in the region between the two spirals.) Then from the assumed asymptotic form of (1), with $\mu = \frac{1}{2}$,

$$c'_n \sim n^{2\alpha+3/4} \exp(a\sqrt{2}\sqrt{n}). \tag{15}$$

Thus the asymptotic behaviour of c'_n takes the same form as that for c_n, except that $\alpha' = 2\alpha + 3/4 = -\frac{5}{4}$ and $a' = a\sqrt{2} \cong 2\pi/\sqrt{3}$ replace α and a. Of course, the size exponent for r'_n remains the same, $\nu' = \nu = \frac{1}{2}$.

As a final check Privman's (1983) data on the whole scroll-like class of SAWs up through $n = 40$ steps may be analysed. The problem is to distinguish at $n \leq 40$ the difference between n-dependences $n^{\alpha'}$ and $\exp[a'(n^{\mu'})]$, which are more comparable than has usually been encountered in SAW problems. Thus we used combinations of c_n values in an attempt to cancel out either one type of dependence or the other. The $n^{\alpha'}$ and $\exp[a(n^{\mu'})]$ dependences, respectively, should be eliminated in the combinations

$$\begin{aligned} A_n &\equiv \ln\left(\ln\frac{n}{n-2}\ln\frac{c'_{n+2}}{c'_n} - \ln\frac{n+2}{n}\ln\frac{c'_n}{c'_{n-2}}\right) \\ B_n &\equiv [n^{\mu'} - (n-2)^{\mu'}]\ln\frac{c'_{n+2}}{c'_n} - [(n+2)^{\mu'} - n^{\mu'}]\ln\frac{c'_n}{c'_{n-2}}. \end{aligned} \tag{16}$$

The expected large n asymptotic behaviour of these combinations is

$$\begin{aligned} A_n &\to \ln[8a'(\mu')^2] + (\mu' - 3)\ln n \\ B_n &\to \alpha\left([n^{\mu'} - (n-2)^{\mu'}]\ln\frac{n+2}{n} - [(n+2)^{\mu'} - n^{\mu'}]\ln\frac{n}{n-2}\right). \end{aligned} \tag{17}$$

A plot of the data for A_n against $\ln n$ lies close anlong a straight line with slope and intercept leading to $\mu' \cong 0.50 \cong \frac{1}{2}$ and $a' \cong 3.6 \cong a\sqrt{2}$, as expected. The plot of the data for B_n with $\mu' = \frac{1}{2}$ involves some scatter of points due to evident oscillations of periods 2 and 6. Nevertheless, these data points consistently approach an asymptotic line through the origin; its slope yields $\alpha' \cong -1.25 \cong -\frac{5}{4}$, as expected. The disagreement with Privman's (1983) estimates is due to his incorrect assumption that $\mu' = 1$.

In conclusion, three types of approaches have been exploited to treat spiral SAWs. Results which we believe to be exact are obtained: $\mu = \nu = \beta = \mu' = \nu' = \beta' = \frac{1}{2}$, $\alpha = -1$, $\alpha' = -\frac{5}{4}$, $a = \pi\sqrt{2/3}$, and $a' = 2\pi/\sqrt{3}$. That the size exponent ν is $\frac{1}{2}$ implies that the spiral SAWs are unusually compact. Further, our value of the enumeration exponent $\mu = \frac{1}{2}$ is reminiscent of a similar exponent arising in the enumeration of maximally compact SAWs in two dimensions (see, e.g., Gordon *et al* 1976, or Schmalz *et al* 1984). The spiral SAWs are confirmed to lie in a universality class distinct from those for other previously considered directed SAWs.

Note added in proof. Recently, A J Guttman and N C Wormald sent us a preprint of a manuscript submitted to *J. Phys. A* in which they obtain a value of $-\frac{7}{4}$ for the exponent, α', in c'_n, in contrast to our value of $-\frac{5}{4}$ which we now believe to be incorrect. The fault in our approach was the assumption that the proportionality factor in (14) was constant rather than varying as $n^{-1/2}$, which results from a more detailed consideration of the Δ's. It is the atypical Δ's of length $n^{1/2}$ at the outer end of the spirals which are important in (14) whereas it is the typical Δ's of finite length in the middle of the spirals which are addressed in the heuristic arguments. We would like to thank Professor Guttman for sending us the preprint of his work prior to publication.

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