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LETTER TO THE EDITOR

# An exact solution for a spiral self-avoiding walk model on the triangular lattice

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**Abstract.** Exact results are derived for the number $s_n$ of spiral self-avoiding walks with $n$ steps on the triangular lattice. In particular, a closed-form expression is presented for the generating function

$$S(x)=\sum_{n=1}^{\infty} s_n x^n.$$

This result is used to establish a complete asymptotic expansion for $s_n$ which is valid as $n\to\infty$.

Recently considerable interest has been shown in the spiral self-avoiding walk (SAW) model on the *square* lattice (Privman 1983, Blöte and Hilhorst 1984, Whittington 1984, Klein *et al* 1984, Redner and de Arcangelis 1984, Guttmann and Wormald 1984, Joyce 1984). In particular, Blöte and Hilhorst (1984) have established the exact generating function for the number $s_n$ of spiral SAWs with $n$ steps, and have also proved that the asymptotic behaviour of $s_n$ is

$$s_n \sim An^{-\gamma}\exp(\lambda n^{1/2}), \tag{1}$$

as $n\to\infty$, where $A=2^{-2}\times 3^{-5/4}\pi$, $\gamma=\frac{7}{4}$ and $\lambda=2\pi/3^{1/2}$. Guttmann and Wormald (1984) have also independently obtained this asymptotic result, and in addition have demonstrated that the relative error in equation (1) is of $O(1/\sqrt{n})$. It was later shown by one of us (Joyce 1984) that the complete asymptotic expansion for $s_n$ has the form

$$s_n \sim An^{-\gamma}\exp(\lambda n^{1/2})\sum_{m=0}^{\infty}\frac{v_m}{n^{m/2}}, \tag{2}$$

as $n\to\infty$. An exact general formula for the coefficients $v_m$, $(m=0,1,2,\ldots)$ was also given. We see from these results that the behaviour of the spiral SAW model is strikingly *different* from the standard SAW model.

Our aim in the present letter is to investigate the properties of a new spiral SAW model on the *triangular* lattice. In this model each step in the SAW must either point in the same direction as the previous step or in a direction rotated anticlockwise by an angle $2\pi/3$ with respect to it. (Note that the first step of each walk is assumed to be the lattice vector $e_1$ shown in figure 1.) The total number of $n$-step spiral SAWs of this type is defined to be $s_n$. For this *triangular* lattice model we shall give an *exact* expression for the basic generating function

$$S(x)=\sum_{n=1}^{\infty} s_n x^n \tag{3}$$

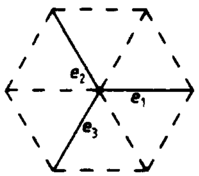


**Figure 1.** Lattice vectors $e_1$, $e_2$, $e_3$.

in terms of the standard generating function

$$Q(x)=\prod_{n=1}^{\infty}(1+x^n)=\sum_{n=0}^{\infty}q(n)x^n, \tag{4}$$

where $q(n)$ is the number of partitions of $n$ into *distinct* parts (see Andrews 1976, p 5). We shall also derive a complete asymptotic expansion for $s_n$ as $n\to\infty$ which has the same *form* as the expansion (2) for the square lattice model.

An $n$-step spiral SAW is made up of a sequence of $L$ line *segments*. The number of single steps in the $i$th segment is denoted by $m_i$, where $i=1,2,\ldots L$ and $m_1+m_2+\ldots+m_L=n$. If the numbers $m_1,\ldots,m_L$ satisfy the inequalities $1\leqslant m_1<m_2<\ldots<m_{L-1}$, $m_L\geqslant 1$, then the walk is said to be an *outward* spiral SAW (see figure 2($a$)).

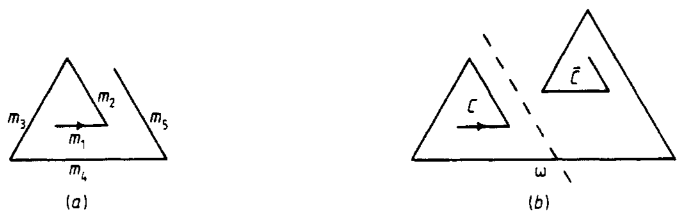


**Figure 2.** ($a$) An outward spiral SAW with segment lengths $m_1\ldots m_5$. ($b$) A trapped spiral SAW which consists of an outward spiral $C$ and an inward spiral $\bar{C}$. The broken dividing line intersects the dividing segment $\omega$.

(Note that every spiral SAW with $L=1$ or $L=2$ is an *outward* spiral walk.) When a spiral SAW with $L\geqslant 3$ does *not* satisfy all the inequalities for $m_1,\ldots,m_L$ it is called a *trapped* spiral SAW. The structure of *any* spiral SAW can be analysed using the idea of a *dividing line* (Blöte and Hilhorst 1984). This is a line parallel to one of the lattice vectors $e_1$, $e_2$ and $e_3$ (see figure 1) which intersects one and only one segment of the walk. An intersected segment of this type which is parallel to the lattice vector $e_i$ is called a *dividing segment* $\omega_i$ (see figure 2($b$)). It is readily seen that the following properties are valid.

(i) Each spiral SAW has either a single dividing segment or two *adjacent* dividing segments.

(ii) In general, a spiral SAW consists of an outward spiral walk $C$ linked by a dividing segment to an inward spiral walk $\bar{C}$ (see figure 2($b$)). If there are two dividing segments this decomposition is clearly not unique. (Note that for a certain subset of spiral SAWs the spiral $C$ will be absent, while for some outward spiral SAWs $\bar{C}$ will not occur.)

We now consider the generating function

$$S^*(x)=\sum_{n=1}^{\infty} s_n^* x^n, \tag{5}$$

where $s_n^*$ is the number of $n$-step *outward* spiral SAWs. To evaluate $S^*(x)$ we use the procedure described by Blöte and Hilhorst (1984). In this manner we obtain

$$S^*(x)=\sum_{m_1=1}^{\infty} x^{m_1}+\sum_{m_1=1}^{\infty}\sum_{m_2=1}^{\infty} x^{m_1+m_2}+\sum_{L=3}^{\infty}\left(\sum_{m_1}\dots\sum_{m_{L-1}}'\right)\sum_{m_L=1}^{\infty} x^{m_1+\dots+m_L}, \tag{6}$$

where the prime on the multiple summation indicates that the integers $m_1,\dots,m_{L-1}$ satisfy the inequalities $1\leqslant m_1<m_2<\dots<m_{L-1}$. We can decouple the restricted summations by introducing the variables $t_i=m_i-m_{i-1}$, $(i=2,3,\dots,L-1)$. The final result is

$$S^*(x)=\frac{x}{1-x}\sum_{k=0}^{\infty} g_k(x), \tag{7}$$

where $g_0(x)\equiv 1$, and

$$g_k(x)=\prod_{i=1}^{k}\left(\frac{x^i}{1-x^i}\right), \qquad (k\geqslant 1). \tag{8}$$

The application of the Euler identity (see Andrews 1976, p 19)

$$1+\sum_{k=1}^{\infty}\frac{z^k x^{k(k+1)/2}}{(1-x)(1-x^2)\dots(1-x^k)}=\prod_{n=1}^{\infty}(1+zx^n), \tag{9}$$

with $z=1$, to equation (7) gives the basic result

$$S^*(x)=\frac{x}{1-x}\prod_{n=1}^{\infty}(1+x^n). \tag{10}$$

It follows from equations (4), (5) and (10) that

$$s_{n+1}^*-s_n^*=q(n), \tag{11}$$

and

$$s_n^*=\sum_{k=0}^{n-1} q(k), \tag{12}$$

where $n\geqslant 1$. The recurrence relation (11) can be used to calculate the values of $s_n^*$ since $q(n)$ has been tabulated for $n\leqslant 400$ by Watson (1937).

Asymptotic representations for $s_n^*$ as $n\to\infty$ can be derived by first analysing the behaviour of $S^*(x)$ in the neighbourhood of its *dominant* singularity $x=1$. We find

$$S^*(x)\simeq 2^{-1/2}[\exp(u)-1]^{-1}\exp[\pi^2/12u)+\tfrac{1}{24}u], \tag{13}$$

as $x\to 1-$, where $u=\ln(1/x)$. (The generating function $S^*(x)$ has *weaker* singularities which form a natural boundary on the circle $|x|=1$.) Next we substitute the standard formula

$$u[\exp(u)-1]^{-1}=\sum_{r=0}^{\infty}\frac{B_r}{r!}u^r, \qquad |u|<2\pi \tag{14}$$

in equation (13), where $B_r$ is a Bernoulli number. If the asymptotic techniques developed by Wright (1933) are applied to each term in the resulting series we eventually obtain the asymptotic expansion

$$s_n^* \sim 2^{-1}3^{1/4}\pi^{-1}n^{-1/4}\exp(\pi n^{1/2}/3^{1/2}) \sum_{m=0}^{\infty} \frac{a_m}{n^{m/2}}, \tag{15}$$

as $n \to \infty$, where

$$a_m = \left(-\frac{3^{1/2}}{2\pi}\right)^m \sum_{t=0}^{m} \sum_{p=0}^{m-t} \frac{(-1)^{p+t}\pi^{2p+2t}B_t}{3^{p+t}p!t!(24)^p}(p+t, m-p-t). \tag{16}$$

In equation (16) the symbol $(\nu, r)$ is defined as

$$(\nu, r) = \frac{1}{2^{2r}r!}(4\nu^2-1)(4\nu^2-3^2)\dots[4\nu^2-(2r-1)^2], \qquad (r \geq 1) \tag{17}$$

with $(\nu, 0) = 1$. The values of the first few coefficients $a_m$ are

$$\begin{aligned} a_0 &= 1, \\ a_1 &= -(\sqrt{3}/144\pi)(11\pi^2-18) \simeq -0.346\,746\,2424, \\ a_2 &= (1/13824\pi^2)(2916+1188\pi^2+73\pi^4) \simeq 0.159\,428\,0738. \end{aligned} \tag{18}$$

When $n = 50$ the truncated expansion (15) gives $s_{50}^* \simeq 27\,924.92$ which agrees well with the exact value $s_{50}^* = 279\,25$.

In order to evaluate the *complete* generating function $S(x)$ we define $S(1, 12, 31; x)$ to be the generating function for the number of all $n$-step spiral SAWs which have just one dividing segment $\omega_1$, or two dividing segments $(\omega_1, \omega_2)$, or two dividing segments $(\omega_3, \omega_1)$. A similar definition holds for the generating function $S(2, 12, 23; x)$ and $S(3, 31, 23; x)$. We also define $S(12; x)$, $S(23; x)$ and $S(31; x)$ to be the generating functions for the number of $n$-step spiral SAWs which have two dividing segments $(\omega_1, \omega_2)$, $(\omega_2, \omega_3)$ and $(\omega_3, \omega_1)$ respectively. From the principle of inclusion and exclusion we readily see that

$$\begin{aligned} S(x) &= S(1, 12, 31; x) + S(2, 12, 23; x) \\ &\quad + S(3, 31, 23; x) - S(12; x) - S(23; x) - S(31; x). \end{aligned} \tag{19}$$

The evaluation of the various $S$-generating functions in equation (19) involves restricted summations of the type (6) over all possible configurations of the outward and inward spirals $C$ and $\bar{C}$ respectively, and over all allowed lengths of the dividing segments. Unfortunately, these calculations are of considerable *complexity* and in this letter we can only give the final expression

$$\begin{aligned} x^4(1-x^3)S(x) &= -(1+2x-2x^3-x^4+x^5+x^6-x^7) + 2(1-x^2)(1+x-x^2-2x^3-x^4+x^5) \\ &\quad \times \prod_{n=1}^{\infty}(1+x^n) - (1-x^2)^2(1-x^2-2x^3)\prod_{n=1}^{\infty}(1+x^n)^2. \end{aligned} \tag{20}$$

The generating function $T(x)$ for the number of $n$-step *trapped* spiral SAWs is clearly given by $S(x) - S^*(x)$.

If we substitute equations (3), (4) and the generating function

$$(Q(x))^2 = \prod_{n=1}^{\infty}(1+x^n)^2 \equiv \sum_{n=0}^{\infty} q_2(n)x^n \tag{21}$$

in equation (20) we obtain the relation

$$\begin{aligned} s_{n+3}-s_n &= 2q_2(n)+q_2(n+1)-4q_2(n+2)-3q_2(n+3)+2q_2(n+4) \\ &\quad +3q_2(n+5)-q_2(n+7)-2q(n)+2q(n+1)+6q(n+2) \\ &\quad -6q(n+4)-4q(n+5)+2q(n+6)+2q(n+7), \end{aligned} \tag{22}$$

where $n \geq 1$, with the initial conditions $s_1 = 1$, $s_2 = 2$ and $s_3 = 3$. The recurrence relation (22) has been used to calculate the exact values of $s_n$ for $n \leq 400$. In table 1 we list the values of $s_n$ for $n \leq 60$. In order to provide a *check* on the basic result (20) a *direct computer* enumeration has been carried out for all spiral SAWs with $n \leq 60$. It was found that the values of $s_n$ obtained in this manner were in *complete agreement* with the results in table 1. Exact closed-form expressions for $q(n)$ and $q_2(n)$ can be derived by applying the methods of Hardy and Ramanujan (1918) and Rademacher (1937) to the generating functions (4) and (21) respectively (see Hua 1942, and Joyce unpublished work).

**Table 1.** Values of $s_n$ for a spiral SAW on the triangular lattice.

| $n$ | $s_n$ | $n$ | $s_n$ | $n$ | $s_n$ |
|---|---|---|---|---|---|
| 1 | 1 | 21 | 945 | 41 | 52 672 |
| 2 | 2 | 22 | 1195 | 42 | 62 658 |
| 3 | 3 | 23 | 1513 | 43 | 74 429 |
| 4 | 5 | 24 | 1882 | 44 | 88 327 |
| 5 | 8 | 25 | 2345 | 45 | 104 524 |
| 6 | 11 | 26 | 2927 | 46 | 123 518 |
| 7 | 17 | 27 | 3608 | 47 | 145 819 |
| 8 | 25 | 28 | 4446 | 48 | 171 737 |
| 9 | 33 | 29 | 5483 | 49 | 201 990 |
| 10 | 47 | 30 | 6701 | 50 | 237 332 |
| 11 | 67 | 31 | 8180 | 51 | 278 289 |
| 12 | 87 | 32 | 9986 | 52 | 325 901 |
| 13 | 117 | 33 | 12 109 | 53 | 381 278 |
| 14 | 160 | 34 | 14 664 | 54 | 445 272 |
| 15 | 207 | 35 | 17 750 | 55 | 519 381 |
| 16 | 270 | 36 | 21 371 | 56 | 605 230 |
| 17 | 356 | 37 | 25 694 | 57 | 704 170 |
| 18 | 455 | 38 | 30 872 | 58 | 818 357 |
| 19 | 584 | 39 | 36 937 | 59 | 950 150 |
| 20 | 751 | 40 | 44 127 | 60 | 1101 634 |

An asymptotic expansion for $s_n$ as $n \to \infty$ can be derived from equation (20) by following the procedure used to obtain expansion (15) for $s_n^*$. The final result is

$$s_n \sim A' n^{-\gamma'} \exp(\lambda' n^{1/2}) \sum_{m=0}^{\infty} \frac{v'_m}{n^{m/2}}, \tag{23}$$

as $n \to \infty$, where $A' = 9^{-1} \times 6^{1/4}\pi$, $\gamma' = \frac{5}{4}$, $\lambda' = 2\pi/6^{1/2}$,

$$\begin{aligned} v'_m = \frac{1}{1152}\left(-\frac{6^{1/2}}{4\pi}\right)^m \sum_{t=0}^{m} \sum_{p=0}^{m-t} \frac{(-1)^{p+t}\pi^{2p+2t}\, 2^{p+t} B_t}{(p+2)!\,t!\,(36)^p}(p+t+2, m-p-t) \\ \times[2+(13)^{p+2}-4(25)^{p+2}-3(37)^{p+2}+2(49)^{p+2}+3(61)^{p+2}-(85)^{p+2}], \end{aligned} \tag{24}$$

and $(\nu, r)$ is defined in equation (17). The values of the first few coefficients $v'_m$ are

$$v'_0 = 1,$$
$$v'_1 = -(5\sqrt{6}/144\pi)(27+2\pi^2) \simeq -1.265\,361\,5137, \qquad (25)$$
$$v'_2 = (7/6912\pi^2)(1215+900\pi^2-404\pi^4) \simeq -3.001\,953\,7875.$$

It can be shown that the *relative* error in formula (23) is the order of $Bn^{1/2}\exp(-\alpha n^{1/2})$, as $n \to \infty$, where $B = -3^{1/2} \times 2^{-1/4}\pi^{-1}$ and $\alpha = \pi(2^{1/2}-1)/3^{1/2}$. When $n = 200$ the truncated expansion (23) yields $s_{200} \simeq 3.703\,18 \times 10^{12}$ which is consistent with the exact value

$$s_{200} = 3702\,615\,665\,774. \qquad (26)$$

It is interesting to note that the dominant asymptotic expansion (23) has the same *structure* as the corresponding result (2) for the *square* lattice, but with different values for the constants $A$, $\gamma$ and $\lambda$.

Finally we note that it is possible to define various other constrained SAW models on the triangular lattice. For example, we can have a spiral SAW model in which the possible anticlockwise rotation angles for the step directions are $(0, \pi/3)$. One could also consider a *mixed* spiral SAW model in which the possible rotation angles for the step directions are $(0, \pi/3, 2\pi/3)$.

We are grateful to Dr D S Gaunt for his continued interest and encouragement in this work, and to Dr A J Guttmann for helpful correspondence. We should also like to thank Mr A L J Wells for carrying out an *independent* numerical calculation of $s_n$ for $n \leqslant 30$. These results provided us with an extremely useful check on the values in table 1. One of us (RB) is grateful to the SERC for the award of a research studentship.

*Note added in proof.* In a recent letter Lin (1985) has also obtained the result (20) for the generating function $S(x)$. However, only the leading-order terms in the asymptotic expansions (15) and (23) are given in this work.

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