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LETTER TO THE EDITOR

An exact formula for the number of spiral self-avoiding walks

G S Joyce

Physics Department, King's College, Strand, London WC2R 2LS, UK

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Abstract. An exact closed-form expression is obtained for the number s_n of spiral self-avoiding walks with n steps on the square lattice. This result is used to derive a complete asymptotic expansion for s_n which is valid as $n \to \infty$.

Recently several authors (Blöte and Hilhorst 1984, Whittington 1984, Klein *et al* 1984, Redner and de Arcangelis 1984) have investigated the properties of a spiral self-avoiding walk model on the square lattice which was first introduced by Privman (1983). A spiral walk is a self-avoiding walk with the additional constraint that the walk is not allowed to make a 90° right-hand turn. (Note that the first step of each walk is assumed to have a *fixed* direction.) Blöte and Hilhorst (1984) have obtained the *exact* generating function for the number s_n of spiral self-avoiding walks with n steps. This generating function was used to show that to *leading-order* the asymptotic behaviour of s_n is

$$s_n \sim 2^{-2} 3^{-5/4} \pi n^{-7/4} \exp(2\pi n^{1/2}/3^{1/2}), \tag{1}$$

as $n \to \infty$.

In this letter we shall express the generating function for s_n in terms of the *standard* generating function

$$P(x) = \prod_{n=1}^{\infty} (1 - x^n)^{-1} = \sum_{n=0}^{\infty} p(n) x^n, \tag{2}$$

where $p(n)$ is the number of unrestricted partitions of n (see Andrews 1976, p 71). An *exact closed-form* expression for s_n is then derived by applying the methods of Hardy and Ramanujan (1918), and Rademacher (1937) to the generating function. This new result is used to establish a *complete* asymptotic expansion for s_n with formula (1) as the leading-order term.

We begin by considering the related generating function

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

where s_n^* is the number of n-step self-avoiding walks which only spiral outward. Blöte and Hilhorst (1984) have shown that

$$S^*(x) = \frac{x}{1-x} \sum_{k=1}^{\infty} g_{k-1}(x)[g_{k-1}(x) + g_k(x)], \tag{4}$$

where $g_0(x)=1$, and

$$g_k(x)=\prod_{i=1}^{k}\left(\frac{x^i}{1-x^i}\right), \qquad (k\geqslant 1). \tag{5}$$

A straightforward rearrangement of equation (4) enables one to write $S^*(x)$ in the alternative form

$$S^*(x)=\frac{x}{1-x}\left(\frac{1}{(1-x)}+\sum_{k=2}^{\infty}\frac{x^{k(k-1)}}{(1-x)^2(1-x^2)^2\ldots(1-x^{k-1})^2(1-x^k)}\right). \tag{6}$$

The application of an identity due to Cauchy (see Andrews 1976, p 20) to equation (6) gives the first simplified formula

$$S^*(x)=\frac{x}{1-x}\prod_{n=1}^{\infty}(1-x^n)^{-1}. \tag{7}$$

It follows from equations (2), (3) and (7) that

$$s_n^*=\sum_{k=0}^{n-1}p(k), \qquad (n\geqslant 1). \tag{8}$$

This formula can be used to calculate the values of s_n^* since the partition function $p(k)$ has been tabulated for $k\leqslant 1000$ by Gupta *et al* (1962). The asymptotic behaviour of s_n^* to leading-order is *readily* determined by applying a general theorem to the infinite product (7), (see Andrews 1976, p 89). We find that the final result agrees with that given by Blöte and Hilhorst (1984).

Next we use the basic formula (7) to simplify the exact expression derived by Blöte and Hilhorst (1984) for the generating function

$$S(x)=\sum_{n=1}^{\infty}s_n x^n, \tag{9}$$

where s_n is the total number of n-step spiral walks. In this manner we obtain

$$x^2S(x)=-(1-x+x^2)-(1-x)(1-2x)\prod_{n=1}^{\infty}(1-x^n)^{-2}+2(1-x)^2\prod_{n=1}^{\infty}(1-x^n)^{-1}. \tag{10}$$

If we substitute equations (2), (9) and the generating function

$$[P(x)]^2=\prod_{n=1}^{\infty}(1-x^n)^{-2}\equiv\sum_{n=0}^{\infty}p_2(n)x^n \tag{11}$$

in equation (10) we obtain the relation

$$s_n=-2p_2(n)+3p_2(n+1)-p_2(n+2)+2p(n)-4p(n+1)+2p(n+2), \tag{12}$$

where $n\geqslant 1$. This result and the table of partitions (Gupta *et al* 1962) enables one to write down the numerical values of s_n for all $n\leqslant 198$. For example,

$$\begin{aligned} s_{65}&=-5506\,157\,680+10\,145\,067\,471-4147\,937\,540\\ &\quad+4025\,116-9294\,080+5359\,378\\ &=491\,062\,665. \end{aligned}$$

This result agrees with the value given by Redner and de Arcangelis (1984). In a similar manner we find

$$s_{100} = 278\,712\,975\,941. \tag{13}$$

From the classic work of Hardy and Ramanujan (1918), and Rademacher (1937) it is known that $p(n)$ can be written as

$$p(n) = \frac{2^{-5/4}3^{-3/4}\pi}{(n-\frac{1}{24})^{3/4}} \sum_{k=1}^{\infty} \frac{A_k(n)}{k} I_{3/2}\left(\frac{\pi}{k}(\tfrac{2}{3})^{1/2}(n-\tfrac{1}{24})^{1/2}\right), \tag{14}$$

where

$$I_{3/2}(z) = \left(\frac{2z}{\pi}\right)^{1/2}\left(-\frac{\sinh z}{z^2} + \frac{\cosh z}{z}\right), \tag{15}$$

is a modified Bessel function of order $\frac{3}{2}$. The coefficients $A_k(n)$ in the series (14) are given by

$$A_k(n) = \sum_{0<h<k}{}' \cos[\pi s(h, k) - (2\pi nh/k)], \qquad (k > 1) \tag{16}$$

with $A_1(n) = 1$, where $s(h, k)$ is the Dedekind sum

$$s(h, k) = \sum_{r=1}^{k-1} \frac{r}{k}\left(\frac{hr}{k} - \left[\frac{hr}{k}\right] - \frac{1}{2}\right), \tag{17}$$

and $[x]$ denotes the greatest integer which is less than or equal to x. The prime in equation (16) indicates that the integers h and k must be coprime.

It should be stressed that equation (14) provides one with an *absolutely convergent* series which can be used to calculate the *exact* numerical value of $p(n)$. In practice we define $T_K(n)$ to be the sum of the truncated series (14) with $k = 1$ to K, and then determine a *rigorous* upper bound $e_K(n)$ for the absolute value of the error $p(n) - T_K(n)$. (Rademacher (1937) has derived various suitable formulae for $e_K(n)$.) The values of $T_K(n)$ are now found for increasing values of $K = 1, 2, \ldots, M$ until there is just *one* integer J in the interval $[T_M(n) - e_M(n), T_M(n) + e_M(n)]$. It is clear that the integer J will give the exact value of $p(n)$. This procedure is illustrated in table 1 for the particular case $p(100)$.

Fortunately, we can also use the Hardy–Ramanujan–Rademacher method to establish an exact convergent series for the coefficient $p_2(n)$ in the generating function (11). The final formula is

$$p_2(n) = \frac{\pi}{6(n-\frac{1}{12})} \sum_{k=1}^{\infty} \frac{B_k(n)}{k} I_2\left(\frac{2\pi}{k\sqrt{3}}(n-\tfrac{1}{12})^{1/2}\right), \tag{18}$$

where

$$B_k(n) = \sum_{0<h<k}{}' \cos[2\pi s(h, k) - (2\pi nh/k)], \qquad (k > 1) \tag{19}$$

with $B_1(n) = 1$ and $n \geq 1$. In equation (19) $s(h, k)$ is a Dedekind sum, and the prime indicates that the integers h and k are coprime. If the basic formulae (14) and (18) are substituted in equation (12) we obtain an exact closed-form expression for the number of spiral walks s_n. The numerical values of $p_2(n)$ have been determined by applying the error bound method to the truncated series (18). In table 1 we list the numerical results for the particular case $p_2(100)$. The closed-form expression for s_n has also been evaluated for $n \leq 150$. Agreement was found with all the available data for s_n (Privman 1983, Blöte and Hilhorst 1984, Redner and de Arcangelis 1984).

Table 1. Evaluation of $p(100)$ and $p_2(100)$ using the closed-form expressions (14) and (18) respectively.

K	$T_K(100)$ for $p(100)$	$e_K(100)$	$T_K(100)$ for $p_2(100)$	$e_K(100)$
1	190 568 944.783	2.2×10^7	1843 645 804 262.089	—
2	190 569 293.655	2.9×10^2	1843 645 820 774.418	6.6×10^4
3	190 569 291.057	1.0×10	1843 645 820 763.904	2.7×10^2
4	190 569 291.742	2.48	1843 645 820 765.611	1.9×10
5	190 569 292.060	1.20	1843 645 820 766.045	4.15
6	190 569 291.996	0.784	1843 645 820 765.980	1.53
7	190 569 292.014	0.592	1843 645 820 766.005	0.767

$p(100)=190\,569\,292$ $\qquad p_2(100)=1843\,645\,820\,766.$

A sequence of *asymptotic* representations for $p(n)$ and $p_2(n)$ can be simply obtained by forming successive truncations of the series (14) and (18) respectively. To *leading-order* we have

$$p(n)\sim\frac{2^{-5/4}3^{-3/4}\pi}{(n-\frac{1}{24})^{3/4}}I_{3/2}[\pi(\tfrac{2}{3})^{1/2}(n-\tfrac{1}{24})^{1/2}], \tag{20}$$

and

$$p_2(n)\sim\frac{\pi}{6(n-\frac{1}{12})}I_2\left(\frac{2\pi}{\sqrt{3}}(n-\tfrac{1}{12})^{1/2}\right), \tag{21}$$

as $n\to\infty$. The relative errors in these asymptotic representations decrease exponentially fast as $n\to\infty$. From these asymptotic results and equation (12) we find that the *dominant* asymptotic representation for s_n is

$$s_n\sim\frac{\pi}{6n}\sum_{m=0}^{2}\frac{a_m}{(1+\varepsilon_{m,n})}I_2[z(1+\varepsilon_{m,n})^{1/2}], \tag{22}$$

as $n\to\infty$, where

$$z=2\pi(n/3)^{1/2}, \tag{23}$$

$$\varepsilon_{m,n}=(m-\tfrac{1}{12})/n, \tag{24}$$

and $a_0=-2$, $a_1=3$, $a_2=-1$. The relative error in the formula (22) is of $O(\exp(-\lambda n^{1/2}))$, with $\lambda=\pi(\sqrt{2}-1)(\frac{2}{3})^{1/2}$. For the particular case $n=100$, the dominant representation (22) gives $s_{100}\simeq2.787\,07\times10^{11}$ which is in good agreement with the exact value (13).

In order to establish a link with the asymptotic analysis of Blöte and Hilhorst (1984) we now apply the Lommel expansion (Watson 1944)

$$\frac{1}{(1+\varepsilon)^{\nu/2}}I_\nu[z(1+\varepsilon)^{1/2}]=\sum_{l=0}^{\infty}\frac{(\varepsilon z/2)^l}{l!}I_{\nu+l}(z), \tag{25}$$

with $\nu=2$ to equation (22). Hence we obtain

$$s_n\sim\frac{\pi}{6n}\sum_{l=0}^{\infty}\left(\frac{3^{-1/2}\pi}{12n^{1/2}}\right)^l\frac{I_{l+2}(z)}{l!}[-2(-1)^l+3(11)^l-(23)^l], \tag{26}$$

as $n\to\infty$, where z is defined in equation (23). Next we substitute the standard asymptotic expansion

$$I_\nu(z) \sim (2\pi z)^{-1/2} e^z \sum_{r=0}^{\infty} (-1)^r (\nu, r)(2z)^{-r} \tag{27}$$

in equation (26), where

$$(\nu, r) = \frac{1}{2^{2r} r!}(4\nu^2 - 1)(4\nu^2 - 3^2) \ldots [4\nu^2 - (2r-1)^2], \qquad (r \geq 1) \tag{28}$$

with $(\nu, 0) = 1$. A rearrangement of the resulting double series yields the basic asymptotic expansion

$$s_n \sim 2^{-2} 3^{-5/4} \pi n^{-7/4} \exp(2\pi n^{1/2}/3^{1/2}) \sum_{m=0}^{\infty} \frac{v_m}{n^{m/2}}, \tag{29}$$

as $n \to \infty$, where

$$v_m = \tfrac{1}{12}\left(-\frac{3^{1/2}}{4\pi}\right)^m \sum_{t=0}^{m} \frac{(-1)^t \pi^{2t} (t+3, m-t)}{(t+1)! 9^t} [2(-1)^t + 3(11)^{t+1} - (23)^{t+1}]. \tag{30}$$

The values of the first few coefficients v_m are

$$\begin{aligned} v_0 &= 1, \\ v_1 &= -\frac{7\sqrt{3}}{144\pi}(45 + 4\pi^2) \simeq -2.264\,081\,5879, \\ v_2 &= \frac{1}{138\,24\pi^2}(76\,545 + 31\,752\pi^2 - 3632\pi^4) \simeq 0.264\,845\,6899. \end{aligned} \tag{31}$$

The *leading-order* term in the expansion (29) for s_n is in agreement with the asymptotic analysis of Blöte and Hilhorst (1984). However, these authors comment on the fact that their asymptotic formula (1) does *not* provide an accurate approximation for the coefficients s_n when $n \leq 50$. In fact when $n = 100$ the formula (1) gives $s_{100} \simeq 3.574 \times 10^{11}$ which does not agree well with the exact value (13). This poor agreement is largely due to the first *correction* term $v_1/n^{1/2}$ in the expansion (29).

I am grateful to Dr D S Gaunt for several useful discussions and for reading through the first version of this letter.

Note added in proof. In a very recent letter Guttmann and Wormald (1984) have independently derived the Blöte–Hilhorst asymptotic formula (1) for s_n, and have also shown that the relative error in equation (1) is of $O(1/\sqrt{n})$. However, their numerical estimate for the correction coefficient $v_1 \simeq -0.7$ is in serious disagreement with the exact value (31).

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