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On the number of spiral self-avoiding walks on a triangular lattice

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Abstract. An elementary derivation of the complete asymptotic expansion for the number S_n of spiral self-avoiding walks with n steps on a triangular lattice is given.

Spiral self-avoiding walks (SSAW) on a square lattice were first introduced by Privman (1983). The asymptotic behaviour of the number S_n of SSAWs with n steps has been studied by several authors (Blöte and Hilhorst 1984, Whittington 1984, Redner and de Arcangelis 1984, Klein *et al* 1984, Guttmann and Wormald 1984, Joyce 1984, Guttmann and Hirschhorn 1984). In particular, Joyce (1984) derived a complete asymptotic expansion for S_n which is valid as $n \to \infty$.

The SSAW problem on a triangular lattice is properly defined as those self-avoiding walks which, at every step, either go straight ahead, turn through 60°, or turn through 120° (both to the left). The simpler problem where 60° deviations are forbidden has recently been solved by Lin (1985), Joyce and Brak (1985) and Liu and Lin (1985). Joyce and Brak (1985) established a complete asymptotic expansion for S_n, using the asymptotic techniques developed by Wright (1933) which are unknown to most physicists. The purpose of the present paper is to describe an elementary derivation using well known techniques.

We first solve the simpler problem of the subclass of SSAW which only spirals outward. We have (Lin 1985, Joyce and Brak 1985)

$$S_n^* = \sum_{k=0}^{n-1} p(k) \tag{1}$$

where S_n^* is the number of n-step SSAWs on a triangular lattice which only spiral outward, and $p(k)$ is the number of all partitions with distinct parts. From the work of Hua (1942), it is known that $p(n)$ can be written as a convergent series whose leading-order term for $n \to \infty$ is (see Andrews 1976, p 82)

$$p(n) \sim \pi(24n+1)^{-1/2} I_1[\pi(48n+2)^{1/2}/12], \tag{2}$$

where

$$I_1(z) = (\mathrm{d}/\mathrm{d}z) I_0(z) = \sum_{n=0}^{\infty} (z/2)^{2n+1}/n!(n+1)! \tag{3}$$

and I_j is a modified Bessel function of order j. The asymptotic expansion of S_n^* is determined from the Euler–Maclaurin sum formula (Bender and Orszag 1978, p 305):

$$\sum_{k=0}^{n} f(k) \sim \int_0^n f(t)\,\mathrm{d}t + \tfrac{1}{2}f(n) + \sum_{t=2}^{\infty} B_t f^{(t-1)}(n)/t!, \tag{4}$$

where the Bernoulli numbers B_t are defined by

$$t/(\mathrm{e}^t - 1) = \sum_{n=0}^{\infty} B_n t^n/n!. \tag{5}$$

We have $B_0 = 1$, $B_1 = -\frac{1}{2}$, $B_2 = \frac{1}{6}$, $B_4 = -\frac{1}{30}$ and $B_{2n+1} = 0$ for $n > 0$. It follows from (2) and (4) that

$$S_n^* = \sum_{k=0}^{n} p(k) - p(n) \sim \int_0^n p_1(k)\,\mathrm{d}k - \tfrac{1}{2}p_1(n) + \sum_{t=2}^{\infty} B_t p_1{}^{(t-1)}(n)/t!, \tag{6}$$

where

$$p_1(n) = \pi^2 2^{-1/2}\,(6x)^{-1} I_1(x) \tag{7}$$

and $x \equiv \pi(n+1/24)^{1/2}/3^{1/2}$. Using the formula (see Gradshteyn and Ryzhik 1965, p 970)

$$(\mathrm{d}/x\,\mathrm{d}x)^m [x^{-n} I_n(x)] = x^{-m-n} I_{m+n}(x), \tag{8}$$

we get

$$\begin{aligned} p_1^{(t-1)}(n) &= 2^{-1/2}(\pi^2/6)^t (\mathrm{d}/x\,\mathrm{d}x)^{t-1}[x^{-1} I_1(x)] \\ &= 2^{-1/2}(\pi^2/6x)^t I_t(x). \end{aligned} \tag{9}$$

We now apply the Lommel expansion (Watson 1944) to equation (9) and obtain

$$\begin{aligned} x^{-t} I_t(x) &= z^{-t}(1+\varepsilon)^{-t/2} I_t[z(1+\varepsilon)^{1/2}] \\ &= z^{-t} \sum_{p=0}^{\infty} (\varepsilon z/2)^p I_{t+p}(z)/p! \end{aligned} \tag{10}$$

where

$$x = z(1+\varepsilon)^{1/2}, \qquad z = \pi(n/3)^{1/2}, \qquad \varepsilon = 1/24n.$$

Hence we get

$$S_n^* \sim 2^{-1/2} \sum_{t=0}^{\infty} \sum_{p=0}^{\infty} B_t (\pi^2/6z)^t (\varepsilon z/2)^p I_{t+p}(z)/p!\,t!. \tag{11}$$

Finally we substitute the asymptotic expansion (Gradshteyn and Ryzhik 1965, p 962)

$$I_n(z) \sim (2\pi z)^{-1/2}\,\mathrm{e}^z \sum_{r=0}^{\infty} (-1)^r (n, r)(2z)^{-r} \tag{12}$$

in equation (11), where $(n, 0) = 0$ and

$$(n, r) = 2^{-2r}(4n^2-1)(4n^2-3^2)\ldots[4n^2-(2r-1)^2]/r! \tag{13}$$

for $r > 0$. The result is (Joyce and Brak 1985)

$$S_n^* \sim (2\pi)^{-1}(3/n)^{1/4} \exp[\pi(n/3)^{1/2}] \sum_{m=0}^{\infty} v_m n^{-m/2} \tag{14}$$

for $n \to \infty$, where

$$v_m = (-3^{1/2}/2\pi)^m \sum_{p=0}^{m} \sum_{t=0}^{m-p} (-\pi^2/3)^{t+p} B_t(t+p, m-t-p)/(24)^p p!\,t!. \tag{15}$$

The corresponding result for SSAWs on a square lattice is

$$S_n^* \sim (4\pi)^{-1}(2/n)^{1/2} \exp[\pi(2n/3)^{1/2}] \sum_{m=0}^{\infty} v'_m n^{-m/2} \tag{16}$$

where

$$v'_m = (-6^{1/2}/4\pi)^m \sum_{p=0}^{m} \sum_{t=0}^{m-p} (-1)^t (\tfrac{2}{3}\pi^2)^{t+p} B_t(\tfrac{1}{2}+t+p, m-t-p)/(24)^p p!\,t!. \tag{17}$$

The first three coefficients are

$$\begin{aligned} v'_0 &= 1, \\ v'_1 &= -13(3/2)^{1/2}\pi/72 \sim -0.6947, \\ v'_2 &= (121\pi^2 + 1872)/6912 \sim 0.4436. \end{aligned} \tag{18}$$

Formula (16) is a new result which has not been reported in the literature.

We now consider the problem of all SSAWs. The generating function is (Lin 1985, Joyce and Brak 1985)

$$G(z) = \sum_n S_n z^n \sim (2z^5 + 5z^4 + 4z^3 - 2z - 1) z^{-4}(1-z)^2(1-z^3)^{-1} g^2(z), \tag{19}$$

where

$$g^2(z) = \left(\sum_{n=0}^{\infty} p(n) z^n \right)^2 \equiv \sum_{n=0}^{\infty} p_2(n) z^n. \tag{20}$$

It can be shown by the Hardy-Ramanujan-Rademacher method (see Andrews 1976, p 68) that to leading order

$$p_2(n) \sim \pi(24n+2)^{-1/2} I_1[\pi(24n+2)^{1/2}/6]. \tag{21}$$

We define

$$(1-z^3)^{-1} g^2(z) = \sum_{n=0}^{\infty} p_3(n) z^n \tag{22}$$

where

$$p_3(n) = p_2(n) + p_2(n-3) + \ldots = \sum_{k=0}^{[n/3]} p_2(3k+h), \tag{23}$$

$h \equiv n - 3[n/3]$, and $[a]$ is the integer part of the number a. We apply the Euler-Maclaurin sum formula to (23) and obtain

$$p_3(n) \sim 6^{-1} \sum_{t=0}^{\infty} (-\pi^2/x)^t I_t(x) B_t/t! \tag{24}$$

where

$$x = z(1+\varepsilon)^{1/2}, \qquad z = \pi(2n/3)^{1/2}, \qquad \varepsilon = 1/12n.$$

It follows from (19) that

$$S_n \sim \sum_{m=-3}^{4} p_3(n+m)a_m \tag{25}$$

where $a_{-3}=2$, $a_{-2}=1$, $a_{-1}=-4$, $a_0=-3$, $a_1=2$, $a_2=3$, $a_3=0$ and $a_4=-1$. Following the same procedure as before, the final result is

$$S_n \sim 2^{1/4}3^{-7/4}\pi n^{-5/4}\exp[\pi(2n/3)^{1/2}]\sum_{m=0}^{\infty} v_m n^{-m/2}, \tag{26}$$

where

$$\begin{aligned} v_m = (1152)^{-1}(-6^{1/2}/4\pi)^m \sum_{p=0}^{m}\sum_{t=0}^{m-p}(-1)^p(2\pi^2)^{p+t}B_t \\ \times(p+t+2, m-p-t)\left(\sum_{s=-3}^{4} a_3(12s+1)^{p+2}\right)/t!(p+2)!(36)^p. \end{aligned} \tag{27}$$

Equation (27) is equivalent to the result of Joyce and Brak (1985) if we make the replacement

$$\sum_{s=-3}^{4} a_s(12s+1)^{p+2} \to (-1)^t \sum_{s=-3}^{4} a_2(12s+37)^{p+2}. \tag{28}$$

The replacement is allowed because of the following identity:

$$\begin{aligned} [u/(e^u-1)]\exp[u(x+36)/36] &= \sum_{t=0}^{\infty}\sum_{p=0}^{\infty} B_t u^{t+p}(x+36)^p/t!p!(36)^p \\ &= [(-u)/(e^{-u}-1)]\exp(ux/36) \\ &= \sum_{t=0}^{\infty}\sum_{p=0}^{\infty}(-1)^t B_t u^{t+p}x^p/t!p!(36)^p. \end{aligned} \tag{29}$$

We were not aware of the work of Joyce and Brak until we finished our derivation.

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