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Number of anisotropic spiral self-avoiding loops†

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Abstract. Two new models of anisotropic spiral self-avoiding loops on the square lattice are considered. These models are closely related to the models of anisotropic spiral self-avoiding walks, which were recently proposed by Manna. The generating function for the number U_n of anisotropic spiral self-avoiding loops with n steps is derived for each model. It is shown that the asymptotic form of U_n (n must be even) is $n^{-1/2}\mu^n$ where μ is the connective constant of the corresponding Manna model.

1. Introduction

Recently Manna (1984) has proposed two models of spiral self-avoiding walk (SSAW) on the square lattice, with spiral constraints after east and west steps but not after north and south steps. We label the four possible steps by N, E, S, W in an obvious notation. In the first model (two-choice anisotropic SSAW), an N (S) step and a W (E) step cannot be followed by an N (S) step. In the second model (three-choice anisotropic SSAW), a W (E) step cannot be followed by an N (S) step. The second model is less restictive than the first model. The asymptotic behaviour of such walks appears to be (Guttmann and Wallace 1986)

$$C_n \sim E\mu^n \exp(\alpha\sqrt{n})n^\beta$$
$$R_n \sim Fn^\nu \tag{1}$$

where $\beta \approx -0.9$, $\nu \approx 0.855$, C_n is the number of distinct n-step walks and R_n is the root mean-square end-to-end distance of all n-step walks. The connective constant is known exactly (Whittington 1985):

$$\begin{aligned}\mu &= (1+\sqrt{5})/2 \qquad &&\text{first model}\\ &=2 &&\text{second model.}\end{aligned} \tag{2}$$

The asymptotic form for the number U_n of self-avoiding loops with n steps is usually written in the form

$$U_n \sim E\mu^n n^h \tag{3}$$

where μ is the connective constant for the self-avoiding walks on a d-dimensional lattice. Notice that this form is not true unless n is suitably restricted. For the square

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lattice, n must be even. The existence of the exponent h has never been established, though it is consistent with numerical evidence. The weaker result that $\log(U_{2n})/(2n)$ converges to μ is due to Hammersley (1961). It has been pointed out by de Gennes (1979) that $h=-d\nu$ where ν is the root mean-square end-to-end distance exponent. What de Gennes has shown by an ingenious but entirely formal argument is that self-avoiding walks are obtained as the degenerate limit of the n-vector model. The scaling laws of equilibrium statistical mechanics thus relate h (if it exists) to ν (if it exists). It is pointed out by Manna (1985) that the scaling relation $h=-d\nu$ is not obeyed by the spiral self-avoiding loops on the square lattice. The scaling relation fails also for spiral self-avoiding loops on the triangular lattice (Lin *et al* 1986). It should be mentioned that the argument of de Gennes about the number of n-step self-avoding loops refers to such loops without the spiral constraint.

The purpose of the present paper is to study anisotropic spiral-self-avoiding loops on the square lattice.

2. The two-choice anisotropic spiral self-avoiding loops

We have studied a new model of anisotropic spiral self-avoiding loops on the square lattice. This model is closely related to Manna's model of two-choice anisotropic spiral self-avoiding walks. In addition to the constraints described in his model, we require that if the first step is N (or S), then the final step before returning to the starting point cannot be W (or E). Exact results are derived for the number U_n of such loops with n steps.

There are four possible steps for the first move. The corresponding generating functions are denoted by G_A where $A=$ N, S, E or W. It is obvious that $G_{\mathrm{N}}=G_{\mathrm{S}}$ and $G_{\mathrm{E}}=G_{\mathrm{W}}$. The overall generating function is

$$G(x)=2[G_{\mathrm{E}}(x)+G_{\mathrm{N}}(x)]$$
$$=\sum_{n=1}^{\infty} U_n x^n. \tag{4}$$

Consider G_{E} first. The constraints restrict the shape of an arbitrary loop to be an r-step staircase. Loops of $r\leqslant 3$ are shown in figure 1. We write

$$G_{\mathrm{E}}(x)=\sum_{r=1}^{\infty} G_r(x) \tag{5}$$

where G_r is the generating function corresponding to all r-step staircases. A loop with $r=1$ and perimeter length $2(m+1)$ (see figure 1) will occur m times, depending on the position of the starting point on the bottom. Therefore we have

$$G_1=\sum_{m=1}^{\infty} m x^{2m+2}=x^4(1-x^2)^{-2}. \tag{6}$$

There are $\binom{m+1}{2}$ ways to construct a loop with $r=2$ and perimeter length $2(m+4)$, and each loop will occur $(m+2)$ times depending on the position of the starting point. Consequently we have

$$G_2=\sum_{m=1}^{\infty}(m+2)\binom{m+1}{2}x^{2(m+4)}$$
$$=3x^{10}(1-x^2)^{-4}. \tag{7}$$

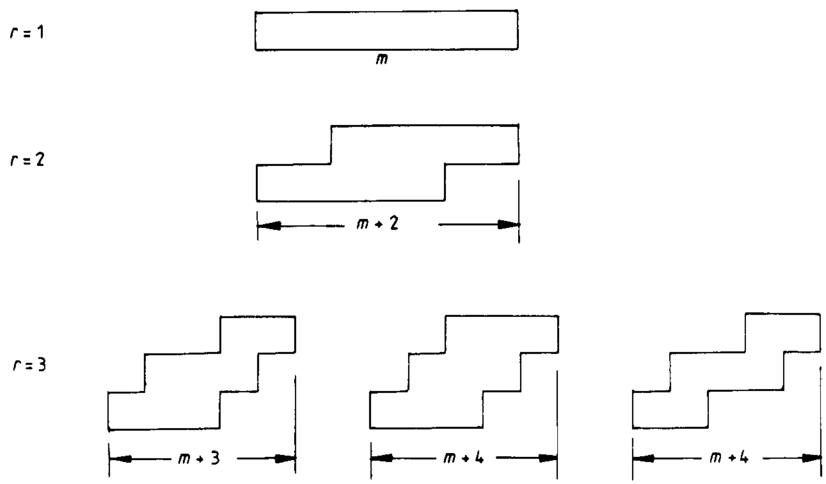

Figure 1. Examples of the first category of anisotropic spiral self-avoiding loops where the starting point can be anywhere around the loop.

There are three different types of loops with $r=3$ (see figure 1) and we have

$$G_3=\sum_{m=1}^{\infty}\left[(m+3)\binom{m+2}{3}x^{2(m+6)}+2(m+4)\binom{m+3}{4}x^{2(m+7)}\right]$$
$$=4x^{14}(1-x^2)^{-5}+10x^{16}(1-x^2)^{-6}. \tag{8}$$

In the general case with $r\geqslant 2$, we have

$$G_r=\sum_{m=1}^{\infty}\sum_{s}(m+s)\binom{m+s-1}{s}F(r,s)x^{2(m+s+r)} \tag{9}$$

where $2r-2\geqslant s\geqslant r$ and

$$F(r,r+k)=[(r-2)(r-3)\dots(r-k-1)][(r+1)(r+2)\dots(r+k)]/k!\,(k+1)!. \tag{10}$$

It follows from the identity

$$\sum_{m=1}^{\infty}(m+s)\binom{m+s-1}{s}y^{m+s}=(s+1)y^{s+1}/(1-y)^{s+2} \tag{11}$$

that

$$G_r=\sum_{s}^{\infty}(s+1)F(r,s)x^{2(r+s+1)}(1-x^2)^{-s-2}. \tag{12}$$

Summing up G_r, we get a surprisingly simple result:

$$G_{\mathrm{E}}(x)=\sum_{n=1}^{\infty}U_{\mathrm{E},n}x^n$$
$$=\tfrac{1}{2}x^2[(1+2x^4-x^6)(1+x^2+x^4)^{-1/2}(1-3x^2+x^4)^{-1/2}-1+x^2]$$
$$=x^4+2x^6+3x^8+7x^{10}+17x^{12}+40x^{14}+97x^{16}+\dots \tag{13}$$

where

$$U_{\mathrm{E},n}\to U\equiv 5^{-1/4}(2\pi n)^{-1/2}\mu^{n-1} \tag{14}$$

as $n\to\infty$, and $\mu=(1+5^{1/2})/2$ is a root of the equation $1-3x^2+x^4=0$. Notice that μ is the connective constant of Manna's model (Whittington 1985).

Consider G_N next. The constraints restrict the loops to be of two categories, as shown in figures 1 and 2. We denote the corresponding generating functions by G_{Ni} $(i=1,2)$. For loops of the first category (see figure 1), each loop corresponding to an r-step staircase occurs r times, depending on the position of the starting point. Following exactly the same procedure as before, we get

$$G_{N1}(x)=\sum_{r=1}^{\infty} G'_r(x) \tag{15}$$

where

$$G'_1=\sum_{m=1}^{\infty} x^{2m+2}=x^4(1-x^2)^{-1}$$

$$G'_r(r>1)=r\sum_{m=1}^{\infty}\sum_{s}\binom{m+s-1}{s}F(r,s)x^{2(m+s+r)}$$
$$=r\sum_{s}F(r,s)x^{2(r+s+1)}(1-x^2)^{-s-1}$$

and $2r-2\geqslant s\geqslant r$. Summing up G'_r, we have

$$\begin{aligned}G_{N1}(x)&=\sum_{n=1}^{\infty} U_{1,n}x^n\\&=\tfrac{1}{2}x^4[1+(1+x^2-x^4)(1+x^2+x^4)^{-1/2}(1-3x^2+x^4)^{-1/2}]\\&=x^4+x^6+x^8+3x^{10}+7x^{12}+16x^{14}+39x^{16}+\ldots\end{aligned} \tag{16}$$

where $U_{1,n}\to U\mu^{-2}$ as $n\to\infty$.

For loops of the first category, their contribution to the total generating function is

$$\begin{aligned}2(G_E+G_{N1})&=\sum_{n=1}^{\infty} nP_nx^n\\&=2x^4-x^2+(x^2+x^4+3x^6-2x^8)(1-2x^2-x^4-2x^6+x^8)^{-1/2}\\&=4x^4+6x^6+8x^8+20x^{10}+48x^{12}+112x^{14}+272x^{16}+\ldots\end{aligned} \tag{17}$$

where P_n is the number of distinct loops with perimeter length n (each loop occurs n times since the starting point can be anywhere around the loop). We have

$$\sum_{n=1}^{\infty} P_nx^n=\tfrac{1}{2}(1-x^2+x^4)-\tfrac{1}{2}(1+x^2+x^4)^{1/2}(1-3x^2+x^4)^{1/2}. \tag{18}$$

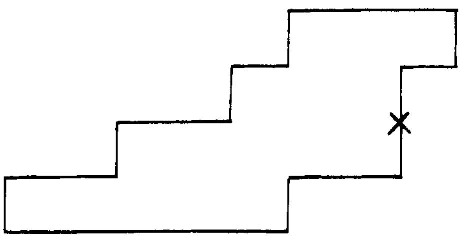

Figure 2. An example of the second category of anisotropic spiral self-avoiding loops where the first step must be a north step and the starting point is unique, as shown by a cross.

For loops of the second category, the first step must be a north step and the starting point is unique. An example is shown in figure 2 where the starting point is marked by a cross. Following the same procedure as before, we obtain

$$G_{N2}(x) = \sum_{r=2}^{\infty} G''_r(x) \tag{19}$$

where

$$G''_r = \sum_{m=1}^{\infty} \sum_{s} \binom{m+s-1}{s} F'(r, s) x^{2(m+s+r)}$$

$$F'(r, r+k-1) = [(r-2)(r-3)\dots(r-k-1)][r(r+1)\dots(r+k-1)]/(k!)^2$$

and $2r-3 \geq s \geq r-1$. Summing up G''_r, we have

$$\begin{aligned} G_{N2}(x) &= \sum_n U_{2,n} x^n \\ &= x^4[(1-x^2+x^4)(1+x^2+x^4)^{-1/2}(1-3x^2+x^4)^{-1/2} - 1]/2 \\ &= x^8 + 2x^{10} + 4x^{12} + 10x^{14} + 24x^{16} + \dots \end{aligned} \tag{20}$$

where $U_{2,n} \to U\mu^{-3}$ as $n \to \infty$.

Finally we have

$$\begin{aligned} G(x) &= 2(G_E + G_{N1} + G_{N2}) \\ &= x^2[x^2 - 1 + (1+2x^2+2x^4-x^6)(1+x^2+x^4)^{-1/2}(1-3x^2+x^4)^{-1/2}] \\ &= 4x^4 + 6x^6 + 10x^8 + 24x^{10} + 56x^{12} + 132x^{14} + 320x^{16} + \dots \\ &= \sum_n U_n x^n \end{aligned} \tag{21}$$

where

$$U_n \to 2(2\pi n)^{-1/2} 5^{-1/4} \mu^n$$

as $n \to \infty$.

If we remove the constraint for the last step before returning to the starting point, then loops of the third category appear. An example is shown in figure 3 where the starting point is marked by a cross. These loops contribute to G_N but not to G_E. Due to the complexity of these loops, we are not able to calculate their contribution.

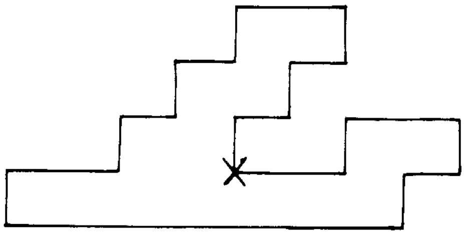

Figure 3. An example of the third category of loops when we remove the constraint for the last step. The starting point is shown by a cross.

3. The three-choice anisotropic spiral self-avoiding loops

A similar model of anisotropic spiral self-avoiding loops is considered. Our model is closely related to Manna's model of three-choice anisotropic SSAW. In his model, a W (E) step cannot be followed by an N (S) step. We further require that if the first step is N (S), then the final step cannot be W (E). These constraints restrict the shape of an arbitrary loop to be a raising staircase followed by a lowering staircase, as shown in figure 4.

The generating function for U_n is

$$G(x)=\sum_{n=1}^{\infty} U_n x^n=\sum nP_n x^n \tag{22}$$

where P_n is the number of distinct loops with perimeter length n. We define

$$S(x,y)=\sum_{r,s=1}^{\infty} P_{r,s}x^s y^r=\sum_{m=1}^{\infty} S_m(x,y) \tag{23}$$

where $P_{r,s}$ is the number of distinct loops with vertical height r and horizontal width s and S_m is the generating function corresponding to all loops whose width at top is m (see figure 4). It is simple to show that

$$S_{m+1}=xS_m+y\sum_{n=0}^{\infty} S_{m+n+1} \tag{24}$$

where $S_0=y$ and $m\geqslant 0$. It follows from equation (24) that

$$S_{m+1}=(1+x-y)S_m-xS_{m-1}. \tag{25}$$

The characteristic equation for the recursion relation (25) is

$$f(z)=z^2-(1+x-y)z+x=(z-z_+)(z-z_-)=0 \tag{26}$$

where

$$z_\pm=\tfrac{1}{2}\{1+x-y\pm[(1+x-y)^2-4x]^{1/2}\}. \tag{27}$$

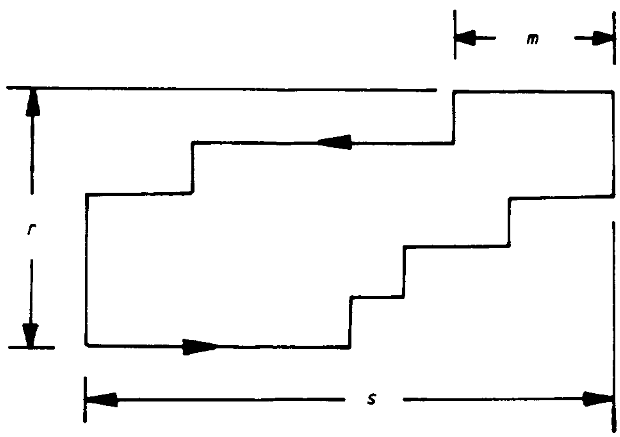

Figure 4. An example of a three-choice anisotropic spiral-self-avoiding loop. The starting point can be anywhere around the loop.

The general solution of equation (25) is

$$S_{m+1} = az_+^m + bz_-^m \tag{28}$$

where

$$a + b = S_1 \qquad az_+ + bz_- = S_2. \tag{29}$$

For $x \to 0$, we have

$$S_m = O(x^m) \qquad z_+ = O(1) \qquad z_- = O(x). \tag{30}$$

Therefore we have $a = 0$ or

$$S_2 = S_1 z_-. \tag{31}$$

It follows from equations (23), (24) and (25) that

$$\begin{aligned} S_1 &= xy + yS \\ S_2 &= xy(x-y) + y(1+x-y)S. \end{aligned} \tag{32}$$

Substituting S_1 and S_2 into equation (31), we obtain

$$S(x, y) = \tfrac{1}{2}\{(1-x-y) - [(1-x-y)^2 - 4xy]^{1/2}\}. \tag{33}$$

Consequently we have

$$\begin{aligned} \sum P_n x^n &= \sum P_{r,s} x^{2(r+s)} = S(x^2, x^2) \\ &= \tfrac{1}{2}[1 - 2x^2 - (1-4x^2)^{1/2}] \\ &= \sum_{n=2}^{\infty} n^{-1} \binom{2n-2}{n-1} x^{2n} \end{aligned} \tag{34}$$

and

$$U_n = nP_n = 2\binom{n-2}{\frac{1}{2}n - 1} = (2n\pi)^{-1/2} 2^n (1 + 3/4n + \ldots) \tag{35}$$

for n(even integers) $\to \infty$. Notice that the connective constant of Manna's model is two (Whittington 1985). Finally we obtain

$$\begin{aligned} G(x) &= (x\, \mathrm{d}/\mathrm{d}x) S(x^2, x^2) \\ &= 2x^2[(1-4x^2)^{-1/2} - 1]. \end{aligned} \tag{36}$$

The first-order correction to the leading term of U_n (see equation (35)) does not support the conjecture that non-integral correction-to-scaling exponents are found in self-avoiding walk problems.

4. Summary

We have studied two new models of anisotropic spiral self-avoidng loops on the square lattice. These models are closely related to Manna's models of anisotropic SSAW. In addition to the constraints described in his two models, we further require that if the first step is N (S), then the final step cannot be W (E). An exact result is derived for the number U_n of n-step loops. It is shown that the asymptotic form of U_n (n must be even) is $n^{-1/2}\mu^n$, where μ is the connective constant of the corresponding Manna model. This asymptotic form is similar to that generally accepted for the number of ordinary self-avoiding polygons, $U_n \propto n^h \mu^n$, where $h = -\frac{3}{2}$ in two dimensions, but the change in the critical exponent should be noted. The scaling relation $h = -d\nu$ connecting the exponent h, the lattice dimension d, and the root mean square displacement exponent ν for self-avoiding walks is destroyed by the anisotropic spiral constraint.

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