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A MODIFIED SELF-AVOIDING WALK MODEL ON THE SQUARE LATTICE WITH REFLECTING AND ABSORBING BARRIERS

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Abstract. Well known is the directed self-avoiding walk model on the square lattice with reflecting and absorbing barriers. We consider two models, namely, a pyramid self-avoiding polygon model and a top and bottom pyramid polygon model, as sub-collections of the model. We derive explicit formulas for the number of $2N$-step polygons in these models.

1. Introduction

An *N-step self-avoiding walk* w on the n-dimensional hypercubic lattice $\mathbb{Z}^d$ is a sequence

$$w = (0 = w(0), w(1), \dots, w(N))$$

with $w(i) \in \mathbb{Z}^d$, $|w(i+1) - w(i)| = 1$ and $w(i) \neq w(j)$ for $i \neq j$. Equal probability is assigned to each N-step self-avoiding walk. A *self-avoiding polygon* is any self-avoiding walk whose final site is a nearest neighbor of the initial site, augmented by the bond joining the final site to the initial site. The self-avoiding walk model was first introduced by chemists as a model of polymer molecules and has been studied by physicists as an interesting model of critical phenomena. Also, it is of interest to probabilists as a natural example of a non Markov process.

The mathematical problems of calculating the exact analytical properties of self-avoiding walks are formidable. In efforts to overcome the difficulties, a number of modified self-avoiding walk models have been actively investigated. It is hoped that the studies on such modified models may shed light on the properties of the full self-avoiding walk model, and provides useful clues on how to approach the extremely difficult self-avoiding walk problem.

Most notable examples are the "spiralling self-avoiding walks" and the "directed self-avoiding walks". In the spiralling self-avoiding walks, turns to specific directions are prohibited, in addition to the self-avoiding condition. In the directed self-avoiding walks, steps to specific directions are prohibited. There are the most obvious shortcoming of the models. In the spiralling self-avoiding walk model, due to the very nature of the model, the walker cannot double back and the resulting walks are very dense

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[1]. Whereas, in the directed self-avoiding walk model, the walker cannot reach certain quarters of the plane: one quarter in "two-choice directed self-avoiding walks" and two quarters in "three-choice directed self-avoiding walks" [6].

Although the self-avoiding polygons are a small collection of the self-avoiding walks, the quantity of the ratio which is obtained by dividing the number of $2N$-step self-avoiding polygons by the number of $2N$-step self-avoiding walks is of particular interest since it represents the probability of return to the origin after $2N$ steps. There are three classes of polygon problems whose exact solutions now exist: these are staircase polygons [5], convex polygons [4] and row-convex polygons [2].

Consider self-avoiding walks in which the walker starts out from the origin and travels over more than two quarters of the plane, winding clockwise around the origin. Such a walk can be divided into several walks that traversed exactly two quarters. Thus, each subwalk that traversed exactly two quarters might be regarded as a "base" of the walk. That is the first reason why we would give a walker "two-choice direction" and "reflecting and absorbing barriers" as microscopic and macroscopic constraint in addition to the self-avoiding condition. On the other hand, "two-choice direction" constraint gives us a model in which most problems can be solved easily and exactly. Moreover, it is possible to derive directly the generating function for the walks consisting of several subwalks that traversed exactly two quarters.

In this paper, we consider a model that the walker may travel over some region on the square lattice with reflecting and absorbing barriers, performing two kinds of two-choice directed self-avoiding walks. The walker starts out from the origin and may take x_+ or y_+ steps until he comes across a reflecting barrier. Thereafter if the walker would arrive at a point of absorbing barrier, he should take x_+ or y_- steps from a reflecting barrier to the last point. Suppose that the walker tries to begin again at the last point and goes on taking his x_- or y_- steps to another reflecting barrier and terminates at a horizontal line below the x-axis with his x_- or y_+ steps. It means that such a walk could be connected with two kinds of two-choice directed self-avoiding walks with reflecting and absorbing barriers. And it is possible for the walker to travel over more than two quarters of the plane. Let the last point be a lattice point that is an intersection of the walks and a horizontal line $y = -1$, in which the walker should pass by the reflecting barrier, and let the endpoint be the origin. Then it becomes a polygon problem. Therefore, we will investigate both a pyramid self-avoiding polygon model and a top and bottom pyramid self-avoiding polygon model.

2. Preliminaries

The generating function $G_1(x_+)$ for one-dimensional self-avoiding walks restrict- ed to the x_+ direction is

$$G_1(x_+) = \frac{1}{1 - x_+} \tag{1}$$

and the generating function $G_2(x_+, y_+)$ for two-choice directed self-avoiding walks in the square lattice in which the walker is restricted only to take either x_+ or y_+ direction is

$$G_2(x_+, y_+) = \frac{1}{1-(x_+ + y_+)}. \tag{2}$$

It follows from (1) and (2) that

$$G_2(x_+, y_+) = G_1(x_+)G_1[y_+G_1(x_+)]. \tag{3}$$

The equation (3) implies that two-choice directed self-avoiding walks in the square lattice are nothing but one-dimensional self-avoiding walks in which the walker is restricted only to take upstairs $[y_+G_1(x_+)](\Rsh)$ direction. Let

$$s_k(x_+, y_+) = G_1(x_+)[y_+G_1(x_+]^k \quad \text{for} \quad k = 0, 1, 2, \ldots, \tag{4}$$

$$T_r(x_+, y_+) = \sum_{k=0}^{r} s_k(x_+, y_+) \quad \text{for} \quad r = 0, 1, 2, \ldots . \tag{5}$$

Thus $s_k(x_+, y_+)$ is the generating function for the walks that start from the horizontal line $y = i$ and reach the horizontal line $y = i + k$. We will use the equation (5) later.

3. Our Model

In this section, we consider a model for two-choice directed self-avoiding walks on the square lattice with reflecting and absorbing barriers. Let the horizontal line $y = r$ be a reflecting barrier and let the horizontal line $y = -m - 1$ be an absorbing barrier, where r and m are nonnegative integers. In this model, the walker who starts out from the origin may take either x_+ or y_+ direction. The walker does or does not visit the reflecting barrier $y = r$. If the walker left the reflecting barrier, he should have taken x_+ direction in the previous step. Once he leaves the reflecting barrier, he must be at a point in the horizontal line $y = r - 1$. Thereafter he may take any of x_+ and y_- directions. If the walker arrived at the absorbing barrier, he should have been in the horizontal line $y = -m$ in the previous step.

The Figure 1 is the diagram of a typical example of a two-choice directed self-avoiding walk on the square lattice with reflecting and absorbing barriers.

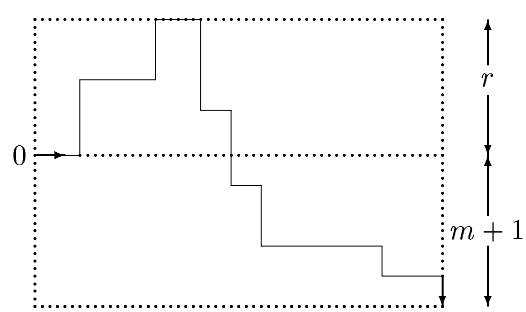

Figure 1. An N-step walk

It follows from the statements above that the generating function for the walks from the origin to the horizontal line $y = -m$ is given by

$$G(x_+, y_+, y_- \,|\, r, -m) = T_r(x_+, y_+) + [s_r(x_+, y_+)]x_+y_-[T_{r+m-1}(x_+, y_-)]$$

if $r \neq 0$, $m \neq 0$ and

$$G(x_+, y_+, y_- \,|\, 0, 0) = T_0(x_+, y_+)$$

and that the generating function for the walks from the origin to the absorbing barrier is given by

$$f(x_+, y_+, y_- \,|\, r, -m-1) = [s_r(x_+, y_+)]x_+y_-[s_{r+m-1}(x_+, y_-)]y_-$$

if $r \neq 0$, $m \neq 0$ and

$$f(x_+, y_+, y_- \,|\, 0, -1) = s_0(x_+, y_+)x_+y_+.$$

Thus the generating function for all walks in the model is

$$U(x_+, y_+, y_- \,|\, r, -m-1) = G(x_+, y_+, y_- \,|\, r, -m) + f(x_+, y_+, y_- \,|\, r, -m-1).$$

Putting $z = x_+ = y_+ = y_-$, we obtain that

$$G(z|\, r, -m) = \begin{cases} \frac{1}{1-2z}\Big(1 - \frac{z^{r+1}}{(1-z)^r} - \frac{z^{2r+m+2}}{(1-z)^{2r+m+1}}\Big) & \text{if } r \neq 0,\, m \neq 0 \\ \frac{1}{1-z} & \text{if } r = 0,\, m = 0, \end{cases}$$

and that

$$f(z|\, r, -m-1) = \frac{z^{2r+m+2}}{(1-z)^{2r+m+1}}.$$

To obtain the number $c_N(r, -m-1)$ of N-step walks, we evaluate the contour integral

$$c_N(r, -m-1) = \frac{1}{2\pi i} \oint \frac{dz}{z^{N+1}} U(z|r, -m-1)$$

along a small circle around the origin. The following identity is well-known (see, for example, [p. 47, 7]):

$$\sum_{k=0}^{n} \binom{r+k-1}{k} 2^{n-k} = \sum_{k=0}^{n} \binom{r+n}{r+k}.$$

Using

$$\lim_{z\to 0} \frac{1}{n!} (\frac{d}{dz})^{(n)} [(1-2z)^{-1}(1-z)^{-r}] = \sum_{k=0}^{n} \binom{r+k-1}{k} 2^{n-k} = \sum_{k=0}^{n} \binom{r+n}{r+k}$$

and

$$2\sum_{k=0}^{n} \binom{r+n}{r+k} - \binom{r+n}{r} = \sum_{k=0}^{n} \binom{r+1+n}{r+1+k},$$

we have a reasonably explicit formula for the number of N-step walks as follows:

$$\begin{aligned} c_N(r,-m-1) = \quad & \binom{N}{0} + \binom{N}{1} + \cdots + \binom{N}{r} \\ + \quad & \binom{N-1}{r+1} + \binom{N-1}{r+2} + \cdots + \binom{N-1}{2r+m} \\ + \quad & \binom{N-2}{2r+m}. \end{aligned}$$

Therefore, if we let $a_N(r,-m-1)$ denote the number of N-step walks that terminate at a lattice point of the absorbing barrier, then we obtain

$$a_N(r,-m-1) = \binom{N-2}{2r+m}. \tag{6}$$

4. Pyramid self-avoiding polygons

In the $(2N-1)$-step walks, the walker starts out from the origin and must pass by some reflecting barrier, $y = r$, to visit the point $(N-r-1,-1)$. Next he should go back to the vertical line $x = 0$ (actually, the point $(0,-1)$) using his remaining $N-r-1$ steps only in the x_- direction. Finally, taking one more step in the y_+ direction, the walker makes a $2N$-step polygon. See a typical example of a $2N$-step polygon in Figure 2.

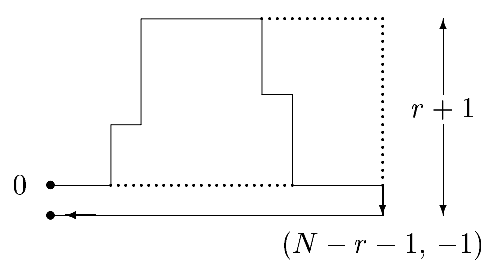

FIGURE 2. A $(2N-1)$-step walk

First, observe that in any of this polygon, the number of x_--steps is just as many as the number of x_+-steps. Substituting x_+x_- for x_+ in $f(x_+,y_+,y_-|\,r,-1)y_+$, summing it up over r from 0 to ∞, putting $z = x_+ = x_- = y_+ = y_-$, we obtain the generating function for the polygons as follows:

$$G^{psap}(z) = \frac{z^4(1-z^2)}{(z^2+z-1)(z^2-z-1)}, \tag{7}$$

with a critical point at $z_c = (\sqrt{5}-1)/2$. Notice that (7) coincides accidentally with one of the results found by Lin et al [4] when they studied convex polygons on the square lattice. Evaluating the residues yields

$$a_N^{psap} = \frac{1-(-1)^{N-3}}{2\sqrt{5}}\Big[\Big(\frac{\sqrt{5}+1}{2}\Big)^{N-3} + \Big(\frac{\sqrt{5}-1}{2}\Big)^{N-3}\Big]$$

for $N \geq 4$.

The following identity is well-known (see, for example, [p. 10, 3]):

$$\sum_{r=0}^{N-2} \binom{N+r-2}{2r} = \frac{1}{\sqrt{5}}\Big[\Big(\frac{\sqrt{5}+1}{2}\Big)^{N-3} + \Big(\frac{\sqrt{5}-1}{2}\Big)^{N-3}\Big], \tag{8}$$

which is the $2(N-2)$-th Fibonacci number. We have seen that

$$\begin{aligned} a_{2N}^{psap} &= \sum_{r=0}^{N-2} a_{N+r}(r,-1) \\ &= \sum_{r=0}^{N-2} \binom{N+r-2}{2r}. \end{aligned}$$

Therefore, the identity (8) holds. This is another way to prove the identity (8).

5. Top and bottom pyramid self-avoiding polygons

Let us consider $2N$ step walks that emanate from the origin, pass by two reflecting barriers $y = r_1$ and $y = r_2$, return to the origin. Such polygons always cross the horizontal line $y = -1$. We want to subdivide such a polygon into two parts, one from the origin to the last point on the line $y = -1$ and another one from the last point on the line to the origin. Suppose that the first part (or top pyramid) has N_1 steps and thus the second part (or bottom pyramid) has $2N - N_1$ steps. And then the last point is just $(N_1 - 2r_1 - 1, -1)$ or $(2N - N_1 - 2r_2 - 1, -1)$.

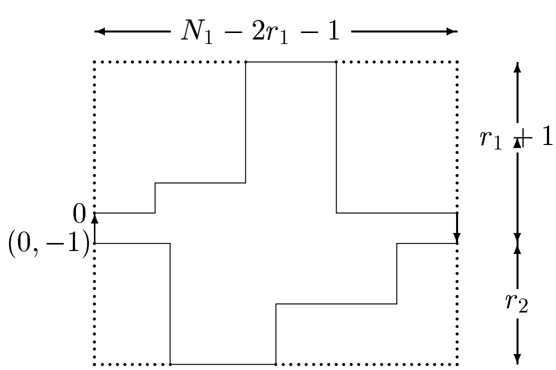

Figure 3. A $2N$-step top and bottom polygon

Then, using equation (6), we have a reasonably explicit formula for the number of $2N$-step polygons as follows:

$$\begin{aligned} a_{2N} &= \sum_{r_1=0}^{N-2} \sum_{r_2=0}^{N-2-r_1} a_{N_1}(r_1,-1)a_{N-N_1}(r_2,-1) \\ &= \sum_{r_1=0}^{N-2} \sum_{r_2=0}^{N-2-r_1} \binom{N+r_1-r_2-2}{2r_1}\binom{N+r_2-r_1-2}{2r_2}. \end{aligned}$$

Here is a table for a_{2N}. The entries for $2N \leq 10$ were verified by drawing all of the diagrams for $2N$-step top and bottom pyramid self-avoiding polygons.

$2N$	a_{2N}
4	1
6	3
8	10
10	36
12	136
14	528
16	2080
18	8256
20	32896
50	35184376283136
100	396140812571323095342603304960

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