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Rigorous results for the number of convex polygons on the square and honeycomb lattices

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Abstract. The generating functions for the number of convex polygons on the square and honeycomb lattices are derived rigorously. These functions were found by Guttmann and Enting. Their calculation is based on the series expansions up to the 64th order and is non-rigorous. The asymptotic form of the mean-squared radius of gyration of n-step convex polygons on the square lattice is determined and the critical exponent ν is 1.

1. Introduction

Convex polygons are defined by Guttmann and Enting (1988b) as self-avoiding polygons whose number of steps equals the perimeter of their minimal bounding rectangle. Any vertical (horizontal) line drawn through the polygon between any two vertices of the graph cuts exactly two horizontal (vertical) bonds. Guttmann and Enting enumerated the number P_n of convex polygons with n steps on the square and honeycomb lattices up to $n=64$. They determined the precise recurrence relation for P_n by systematic searching and then obtained the exact solution of the recurrence relation in a closed form. Their calculation of the generating function

$$P(x)=\sum_{n=2}^{\infty} P_{2n}x^{2n} \qquad (1)$$

is non-rigorous because they did not derive the recurrence relation rigorously.

Recently a method has been developed by Ma and Lin (1988) to calculate the number of anisotropic spiral self-avoiding loops. In the present paper we apply the method of Ma and Lin to derive rigorously the generating function for the number of convex polygons.

2. Convex polygons on the square lattice

Consider first a special case of convex polygons as shown in figure 1. The width at the top of such a polygon equals the width of the minimal bounding rectangle. The generating function for the number $G_{r,s}$ of convex polygons with vertical height r and horizontal width s is

$$G(x^2,y^2)=\sum_{r,s=1}^{\infty} G_{r,s}y^{2r}x^{2s}=\sum_{m=1}^{\infty} G_m \qquad (2)$$

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where

$$G_m = x^{2m} \sum_{r=1}^{\infty} G_{r,m} y^{2r} \tag{3}$$

is the generating function corresponding to all polygons whose width at the top is m.

By considering the addition of the top row of squares in figure 1, it is easy to show that

$$G_m = y^2 x^{2m} + y^2 \sum_{n=1}^{m} (m+1-n) G_n x^{2(m-n)} \tag{4}$$

whence

$$G_{m+1} - x^2 G_m = y^2 \sum_{n=1}^{m+1} G_n x^{2(m+1-n)} \tag{5}$$

and

$$G_1 = x^2(y^2 + y^4 + \ldots) = x^2 y^2/(1-y^2). \tag{6}$$

It follows from equation (5) that

$$(1-y^2) G_{m+2} - 2x^2 G_{m+1} + x^4 G_m = 0. \tag{7}$$

The characteristic equation for the recursion relation (7) is

$$f(z) = (1-y^2) z^2 - 2x^2 z + x^4 = 0 \tag{8}$$

and the solution is

$$z = z_\pm = x^2/(1 \pm y). \tag{9}$$

The general solution of equation (7) is

$$G_m = a z_+^m + b z_-^m. \tag{10}$$

The coefficients a and b are determined from G_1 and

$$G_2 = x^2 G_1 + y^2 (G_2 + G_1 x^2) \tag{11}$$

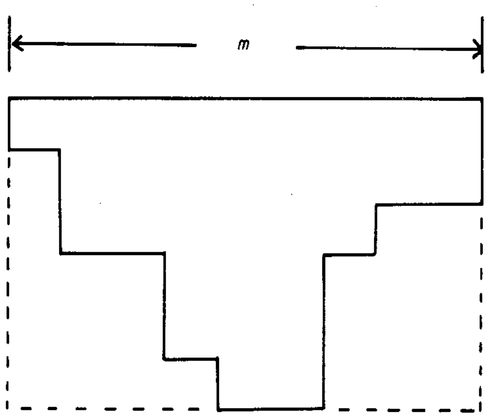

Figure 1. A convex polygon whose width at the top equals the width of the minimal bounding rectangle.

or

$$G_2 = x^2(1+y^2)G_1/(1-y^2) = x^4y^2(1+y^2)/(1-y^2)^2. \tag{12}$$

The result is $a = b = y^2/2$. The generating function is

$$G = x^2y^2(1-x^2)[(1-x^2)^2 - y^2]^{-1}. \tag{13}$$

Consider next the second special case of the convex polygons as shown in figure 2. The top right-hand corner of the minimal bounding rectangle is also a corner of the polygon. Notice that the first special case is a subset of the second one. The generating function is

$$H(x^2, y^2) = \sum_{r,s=1}^{\infty} H_{r,s}y^{2r}x^{2s} = \sum_{m=1}^{\infty} H_m \tag{14}$$

where H_m is the generating function for polygons whose width at the top is m.

In a similar manner to the derivation of (4), we have

$$H_m = y^2x^{2m} + y^2 \sum_{n=0}^{\infty}\sum_{r=1}^{m} H_{n+r}x^{2(m-r)} + y^2 \sum_{n=1}^{m-1}(m-n)G_nx^{2(m-n)} \tag{15}$$

whence

$$H_{m+1} - x^2H_m = y^2 \sum_{n=0}^{\infty} H_{m+n+1} + y^2 \sum_{n=1}^{m} G_nx^{2(m+1-n)}. \tag{16}$$

It follows from (10) and (16) that

$$H_{m+2} - (1+x^2-y^2)H_{m+1} + x^2H_m = c_+z_+^m + c_-z_-^m \tag{17}$$

where

$$c_\pm = \pm x^2y^3(1-x^2\pm y)/2(1\pm y).$$

The characteristic equation for the recursion relation (16) is

$$f(\omega) = \omega^2 - (1+x^2-y^2)\omega + x^2 = 0 \tag{18}$$

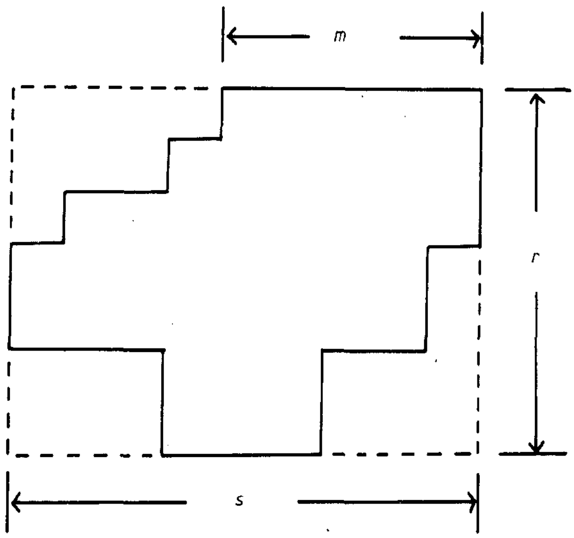

Figure 2. A convex polygon whose top right-hand corner is also the corner of the minimal bounding rectangle.

and the solution is

$$\omega=\omega_{\pm}=\tfrac{1}{2}\{1+x^2-y^2\pm[1-2x^2-2y^2+(x^2-y^2)^2]^{1/2}\}. \tag{19}$$

Notice that (18) and (19) are the same as the equations found by Lin *et al* (1987) when they studied anisotropic spiral self-avoiding loops. The general solution of equation (17) is

$$H_{m+1}=d_+z_+^m+d_-z_-^m+e\omega_+^m+f\omega_-^m \tag{20}$$

where

$$d_{\pm}=x^2y^2(1\pm y-x^2)/2(1\pm 2y+y^2-x^2).$$

When $x\to 0$, we have

$$\begin{aligned} &H_m=O(x^{2m}) \qquad &z_{\pm}=O(x^2)\\ &\omega_+=O(1) \qquad &\omega_-=O(x^2). \end{aligned} \tag{21}$$

Therefore we have $e=0$ and

$$\begin{aligned} H_1&=d_++d_-+f\\ H_2&=d_+z_++d_-z_-+f\omega_-. \end{aligned} \tag{22}$$

It follows from (16) that

$$H_1-H_2=(y^2-x^2)H_1+x^2y^2-x^4y^4/(1-y^2). \tag{23}$$

Substituting H_1 and H_2 into (23), we have

$$f=-2x^2y^4\omega_-[1-2x^2-2y^2+(x^2-y^2)^2]^{-1}. \tag{24}$$

Summing over H_m, we have

$$H=x^2y^2[1-2x^2-2y^2+(x^2-y^2)^2]^{-1/2}. \tag{25}$$

The generating function $P(x^2,y^2)$ for all convex polygons can be determined by the method of Ma and Lin (1988). Each polygon is divided uniquely into two (top and bottom) polygons as shown in figure 3 by a broken line. For the top polygon, the width at botom equals the width of the corresponding minimal bounding rectangle

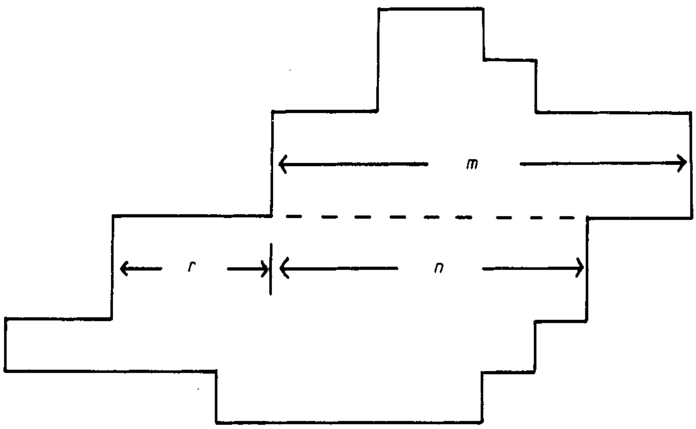

Figure 3. A convex polygon divided into two polygons (top and bottom) by the broken line.

(the first special case). The broken line is chosen such that the top polygon has the maximum area. It can be shown that

$$P(x^2, y^2) = \sum_{r,s=1}^{\infty} P_{r,s} y^{2r} x^{2s}$$
$$= G + 2 \sum_{m=2}^{\infty} G_m \sum_{n=1}^{m-1} x^{-2n} \sum_{p=0}^{\infty} H_{n+p} + \sum_{m=3}^{\infty} G_m \sum_{n=1}^{m-2} G_n x^{-2n}(m-n-1). \quad (26)$$

The first term on the RHS corresponds to the special case where the bottom polygon reduces to a line. A factor of two in the second term is due to the fact that each polygon as shown in figure 3 corresponds one-to-one with another polygon which is obtained from the original one by reflection along the vertical direction. The last term corresponds to polygons as shown in figure 4. The factor $(m-n-1)$ is the number of ways to connect the top and bottom polygons within the same minimal bounding rectangle. After a straightforward calculation, we obtain

$$P(x^2, y^2) = x^2y^2[1 - 3x^2 - 3y^2 + 3x^4 + 3y^4 + 5x^2y^2 - x^6 - y^6 - x^2y^4$$
$$- x^4y^2 - x^2y^2(x^2 - y^2)^2]\Delta^{-2} - 4x^4y^4\Delta^{-3/2} \quad (27)$$

where

$$\Delta = 1 - 2x^2 - 2y^2 + (x^2 - y^2)^2.$$

When $x = y$ we obtain

$$P(x^2) = \sum_{m=2}^{\infty} P_{2m} x^{2m}$$
$$= x^4(1 - 6x^2 + 11x^4 - 4x^6)(1 - 4x^2)^{-2} - 4x^8(1 - 4x^2)^{-3/2}$$
$$= x^4 + 2x^6 + 7x^8 + 28x^{10} + \dots \quad (28)$$

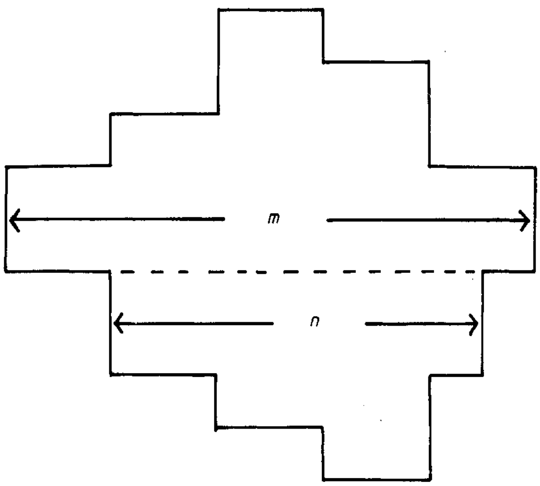

Figure 4. A convex polygon whose top polygon is wider than the bottom one. The minimal bounding rectangle does not contact the two corners at the top side of the bottom polygon.

which was first calculated non-rigorously by Guttmann and Enting (1988b). It follows from (28) that for large n

$$P_n \to n2^{n-8}[1-8(2n\pi)^{-1/2}+\ldots]. \tag{29}$$

We denote the sum of the mth power of the spans of all convex polygons with n steps in a given lattice direction by $D_n^{(m)}$. The mth moment of the caliper size is defined by

$$\langle R_n^m \rangle = D_n^{(m)}/P_n. \tag{30}$$

The radius of gyration is defined by

$$R_n = \langle R_n^2 \rangle^{1/2}. \tag{31}$$

For large n one expects $\langle R_n^m \rangle \sim n^{m\nu}$.

It follows from (26) and (27) that

$$\begin{aligned}\sum_{n=2}^{\infty} D_n^{(m)} x^n &= \sum_{r,s=1}^{\infty} s^m P_{r,s} y^{2r} x^{2s}\big|_{x=y} \\ &= [x^2\delta/\delta(x^2)]^m P(x^2, y^2)\big|_{x=y} \\ &= x^4(1-6x^2+11x^4-4x^6)(m+1)!/2^m(1-4x^2)^{m+2} \\ &\quad -4x^8(2m+1)!!/2^{2m}(1-4x^2)^{m+3/2}+\ldots.\end{aligned} \tag{32}$$

For large n, we have

$$\begin{aligned}D_n^{(m)} &= n^{m+1}2^{n-2m-8}[1-8(2n\pi)^{-1/2}+\ldots] \\ \langle R_n^m \rangle &= (n/4)^m[1+\mathrm{O}(n^{-1})].\end{aligned} \tag{33}$$

The asymptotic form of the radius of gyration is

$$R_n = (n/4)[1+\mathrm{O}(n^{-1})] \tag{34}$$

and the critical exponent ν is 1.

In the special case of $m=1$, we have the exact result

$$\langle R_n \rangle = n/4. \tag{35}$$

Equation (35) follows from the fact that a convex polygon with height r and width s can be transformed into a polygon with height s and width r by rotation and therefore we have $\langle R_n \rangle = (r+s)/2 = n/4$.

Recently Guttmann and Enting (1988a) calculated the number of self-avoiding polygons on the square lattice to 56 steps, and the caliper size to 54 steps. Analysis of the generating functions permits the following estimates of the connective constant μ and the critical exponents α and ν:

$$\mu \sim 2.638 \qquad \alpha \sim 0.5 \qquad \nu \sim 0.75. \tag{36}$$

The corresponding values for the convex polygons are

$$\mu = 2 \qquad \alpha = 4 \qquad \nu = 1. \tag{37}$$

3. Convex polygons on the honeycomb lattice

Following Guttmann and Enting (1988b), the honeycomb lattice is treated as a square lattice with half the vertical bonds missing (the brick wall lattice). We use the same procedure and notations as before. They pointed out that the definition of convexity (cutting any horizontal or vertical line at most twice) refers to the square lattice representation that is used in the algebraic enumeration techniques. This definition of convexity has no natural interpretation on the honeycomb lattice. For this reason we do not consider the size of convex polygons on the honeycomb lattice.

Consider first the special case where the width at the top of each polygon equals the width of the minimal bounding rectangle. We have (m and n are even integers):

$$G_{m+2} = x^4 G_m + y^2 \sum_{n=2}^{m} x^{2(m+2-n)} G_n \tag{38}$$

where

$$G_2 = x^4 y^2 \qquad G_4 = x^8(y^2 + y^4).$$

The recursion relation is (m must be even):

$$G_{m+4} - x^4(2+y^2) G_{m+2} + x^8 G_m = 0. \tag{39}$$

The solution is

$$G_m = x^2 y^2 (4+y^2)^{-1/2} (z_+^{m-1} + z_-^{m-1}) \tag{40}$$

where

$$z_\pm = x^2[(4+y^2)^{1/2} \pm y]/2$$

are the roots of the characteristic equation

$$z^4 - x^4(2+y^2) z^2 + x^8 = 0. \tag{41}$$

The generating function is

$$G = \sum_{m=2}^{\infty} G_m = \frac{x^4 y^2 (1-x^4)}{1 - 2x^4 - x^4 y^2 + x^8}. \tag{42}$$

Consider next the convex polygons whose top right-hand corner is also the corner of the minimal bounding rectangle. We have

$$H_{m+2} = x^4 H_m + x^2 y^2 \sum_{n=0}^{\infty} H_{m+n+2} + y^2 \sum_{n=2}^{m} G_n x^{2(m+2-n)} \tag{43}$$

where m and n are even integers. The recursion relation is

$$\begin{aligned} H_{m+4} - (1 + x^4 - x^2 y^2) H_{m+2} + x^4 H_m \\ = x^4 y^3 [z_+^m (z_+^2 - 1) - z_-^m (z_-^2 - 1)](4+x^2)^{-1/2}. \end{aligned} \tag{44}$$

The solution of equation (44) is

$$H_{m+2} = a t^{m/2} + b_+ z_+^m + b_- z_-^m \tag{45}$$

where

$$2t = 1 + x^4 - x^2 y^2 - [(1 + x^4 - x^2 y^2)^2 - 4x^4]^{1/2}$$

$$a = -x^4y^4t/(1+x^2)(1-2x^2+x^4-x^2y^2)$$

$$b_\pm = \frac{x^4y^2[1-x^2-x^4+x^6-x^4y^2 \pm y(1+x^2-3x^4+x^6-x^4y^2)(4+y^2)^{-1/2}]}{2(1+x^2)(1-2x^2+x^4-x^2y^2)}$$

and t is a root of the characteristic equation

$$t^2-(1+x^4-x^2y^2)t+x^4=0 \tag{46}$$

with the property $t=O(x^4)$ for $x \to 0$. The generating function is

$$H = \sum_{m=2}^{\infty} H_m = \frac{x^2y^2[(1+4x^2/\Delta)^{1/2}-1]}{2(1+x^2)} \tag{47}$$

where $\Delta = (1-x^2)^2 - x^2y^2$.

Finally the generating function of all convex polygons is (m, n and r are even integers):

$$P = G + 2\sum_{m=2}^{\infty} G_m \sum_{n=2}^{m} x^{-2(n-1)} \sum_{r=0}^{\infty} H_{n+r} + \sum_{m=4}^{\infty} G_m \sum_{n=2}^{m-2} G_n x^{-2n}(m-n)/2$$

$$= \frac{x^4y^2[1-2x^2+x^2y^2+2x^6-2x^4y^2-x^8+x^6y^2-x^4y^4-x^2y^2(\Delta\Delta')^{1/2}]}{(1+x^2)^2\Delta^2} \tag{48}$$

where $\Delta' = (1+x^2)^2 - x^2y^2$. When $x=y$ we have

$$P(x^2) = x^6[1-2x^2+x^4-x^8-x^4(1-4x^4)^{1/2}][(1+x^2)(1-2x^2)]^{-2}$$

$$= x^6+3x^{10}+2x^{12}+10x^{14}+14x^{16}+40x^{18}+\ldots \tag{49}$$

which was first derived non-rigorously by Guttmann and Enting (1988b).

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