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Number of almost-convex polygons on the square lattice

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Abstract. The generating function for the number $N_{c,n}$ of almost-convex polygons on the square lattice with concavity index $c = 1$ and perimeter n is derived rigorously. The asymptotic behaviour of $N_{c,n}$ for large n is determined and our result confirms a recent conjecture by Enting *et al.*

1. Introduction

Self-avoiding polygons on regular lattices have been considered as a model of crystal growth (Temperley 1952) or polymer (Temperley 1956, de Gennes 1979). The problem is to determine the generating function for the number of polygons on a lattice with given perimeter and/or area. The problem is very difficult and an exact solution is still unknown. However several restricted classes of polygons can be enumerated and a large amount of exact results were obtained during last few years. These recent developments were reviewed by Guttmann (1991) and Lin (1991b).

Very recently, Enting *et al* (1991) introduced a class of polygons referred to as almost-convex. They defined a concavity index c for polygons on the square lattice by associating with each n -step polygon a minimal bounding rectangle of perimeter m such that $c = (n - m)/2$. The unrestricted polygons consist of almost-convex polygons whose concavity indices vary from zero to infinity. An almost-convex polygon with index $c = n$ can be obtained from a polygon with index $c = n - 1$ by removing a $m \times 1$ or $1 \times m$ rectangle. The number of polygons with concavity c and perimeter n is denoted by $N_{c,n}$. They proved that for $c = O(n^{2/3})$

$$N_{c,n} \approx N_0 \equiv 2^{n-2c-8} n^{c+1} \exp(c^2/n)/c!. \quad (1)$$

They also calculated $N_{c,n}$ up to 60 steps for $c = 1, \dots, 10$ and conjectured that

$$N_{c,n} \approx N_0 [1 - 4(2/n\pi)^{1/2} + O(1/n)]. \quad (2)$$

Convex polygons correspond to $c = 0$. The perimeter generating function for convex polygons was first derived by Delest and Viennot (1984) and then rederived later by different methods (Kim 1988, Guttmann and Enting 1988, Lin and Chang 1988). The area and perimeter generating function for convex polygons was derived independently by Lin (1991a) and Bousequet-Melou (1991). We consider polygons with $c = 1$ in the present paper and derive the generating function for the number of polygons rigorously. The conjecture (2) is verified for $c = 1$. Note that equation (2) also holds for $c = 0$ (Lin and Chang 1988, Enting *et al* 1991).

2. Polygons with concavity one

Consider a polygon on the square lattice with concavity one. Such a polygon can be obtained from a convex polygon by removing a $m \times 1$ ($1 \times m$) rectangle from the right or left (top or bottom) side as shown in figure 1. The generating function for the number N_n of such polygons with perimeter n is defined by

$$G(x) = G_r + G_l + G_t + G_b = \sum_{n=12}^{\infty} N_n x^n \tag{3}$$

where G_r (G_l, G_t, G_b) generates polygons which correspond to removing a rectangle from the right (left, top, bottom) side of convex polygons. It follows from symmetry that $G_r = G_l = G_t = G_b$.

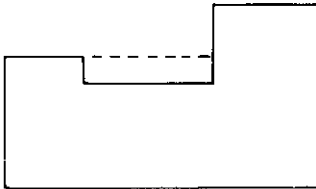


Figure 1. A polygon with concavity one can be obtained from a convex polygon on the square lattice by removing a $1 \times n$ rectangle from the top side.

We shall consider the more general case of rectangular lattice in the present paper. We define a concavity c for polygons on the rectangular lattice by associating with each $2n$ -step polygon an $r \times s$ minimal bounding rectangle such that $c = n - r - s$. The generating function for polygons with $c = 1$ is defined by

$$G(x, y) = G_r(x, y) + G_l(x, y) + G_t(x, y) + G_b(x, y) = \sum_{r=2}^{\infty} \sum_{s=2}^{\infty} N_{r,s} y^{2r} x^{2s} \tag{4}$$

where $N_{r,s}$ is the number of polygons associated with an $r \times s$ minimal bounding rectangle. It follows from symmetry that

$$G_r(x, y) = G_l(x, y) = G_t(y, x) = G_b(y, x). \tag{5}$$

Therefore we shall study $G_t(x, y)$ only from now on.

3. Generating function

A polygon with $c = 1$ can be obtained by placing one $1 \times n$ rectangle and a top convex polygon on the top row of the main convex polygon as shown in figure 2.

The generating functions for several classes of convex polygons are summarized as follows. A pyramid polygon is a special case of convex polygon such that the width at the bottom equals the width of the bounding rectangle. The generating function

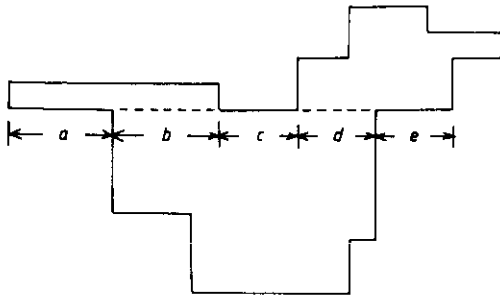


Figure 2. The first special case of polygons with concavity one where the top polygon is an inverse corner polygon and the main polygon is an inverse pyramid polygon.

$P(x, y)$ for the number $P_{r,s}$ of pyramid polygons associated with an $r \times s$ minimal bounding rectangle is

$$\begin{aligned}
 P(x, y) &= \sum_{r,s=1}^{\infty} P_{r,s} y^{2r} x^{2s} = \sum_{m=1}^{\infty} P_m \\
 &= x^2 y^2 (1 - x^2) / [(1 - x^2)^2 - y^2]
 \end{aligned}
 \tag{6}$$

where

$$P_m = y^2 (u_+^m + u_-^m) / 2$$

with

$$u_{\pm} = x^2 / (1 \pm y)$$

generates polygons whose bottom-width is m (Lin and Chang 1988). Another special case of the convex polygon is a polygon whose top right-hand corner of the bounding rectangle is also the corner of the polygon. We shall call them corner polygons. The generating function $H(x, y)$ for the number $H_{r,s}$ of such polygons associated with an $r \times s$ minimal bounding rectangle is

$$H(x, y) = \sum_{r,s=1}^{\infty} H_{r,s} y^{2r} x^{2s} = \sum_{m=1}^{\infty} H_m = x^2 y^2 / \Delta^{1/2}
 \tag{7}$$

where

$$\begin{aligned}
 \Delta &= 1 - 2x^2 - 2y^2 + (x^2 - y^2)^2 \\
 H_m &= (A_+ u_+^m + A_- u_-^m) + A w^m
 \end{aligned}
 \tag{8}$$

with

$$\begin{aligned}
 A_{\pm} &= y^2 (1 \pm y) (1 \pm y - x^2) / 2 [(1 \pm y)^2 - x^2] \\
 A &= -2x^2 y^4 / \Delta \\
 w &= (1 + x^2 - y^2 - \Delta^{1/2}) / 2
 \end{aligned}$$

and H_m generates polygons whose width at the top row is m (Lin and Chang 1988). The generating function $R(x, y)$ for the number $R_{r,s}$ of convex polygons associated with an $r \times s$ minimal bounding rectangle is (Delest and Viennot 1984, Kim 1988, Guttmann and Enting 1988, Lin and Chang 1988)

$$\begin{aligned}
 R(x, y) &= \sum_{r,s=1}^{\infty} R_{r,s} y^{2r} x^{2s} = \sum_{m=1}^{\infty} R_m \\
 &= x^2 y^2 [1 - 3(x^2 + y^2) + 3(x^4 + y^4) + 5x^2 y^2 - x^6 - y^6 \\
 &\quad - x^2 y^4 - x^4 y^2 - x^2 y^2 (x^2 - y^2)^2] / \Delta^2 - 4x^4 y^4 / \Delta^{3/2} \tag{9}
 \end{aligned}$$

where

$$R_m = (D_+ u_+^m + D_- u_-^m) / 2\Delta^2 + E w^m / \Delta^{3/2}$$

with

$$\begin{aligned}
 D_{\pm} &= y^2 (1 \pm y)^2 (1 \pm y - x^2)^2 [(1 \mp y)^2 - x^2]^2 \\
 E &= -2x^2 y^4 (1 - x^2 - y^2 + \Delta^{1/2})
 \end{aligned}$$

and R_m generates convex polygons whose width at the top row is m (Lin 1991c).

The generating function $G_1(x, y)$ for polygons with $c = 1$ can be derived as follows. Consider first the case where the main polygon is an inverse pyramid and the top polygon is an inverse corner polygon as shown in figure 2. The generating function for such polygons is

$$G_1(x, y) = \sum_{a,b,c,d,e=1}^{\infty} y^2 x^{2a} P_{b+c+d} [2(x^{-2d} H_{d+e}) - y^2 x^{2e}]. \tag{10}$$

The factor of two is due to the fact that there are two ways to put the $1 \times n$ rectangle on the top of the main polygon (left-hand or right-hand side). The special configuration where the top polygon degenerates into a $1 \times m$ rectangle has been counted twice and therefore we subtract the corresponding term in the summation.

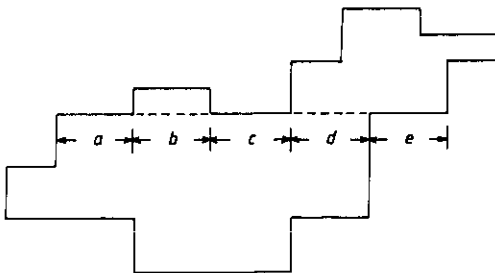


Figure 3. The second special case of polygons with concavity one where the top polygon is an inverse corner polygon and the main polygon is a corner polygon.

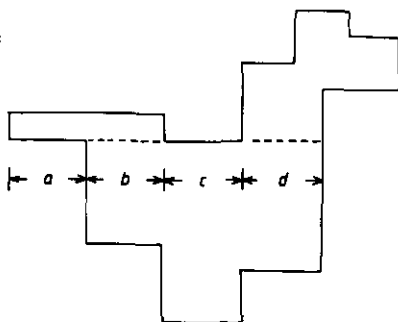


Figure 4. The third special case of polygons with concavity one where the top polygon is an inverse corner polygon (but not pyramid polygon) and the main polygon is an inverse pyramid polygon.

Consider the second case as shown in figure 3 where the top polygon is an inverse corner polygon and the main polygon is a corner polygon. The generating function is

$$G_2(x, y) = 2y^2 \sum_{a=0}^{\infty} \sum_{b,c,d,e=1}^{\infty} x^{-2d} H_{a+b+c+d} H_{d+e}. \tag{11}$$

The factor of two 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.

Consider the third case as shown in figure 4 where the main polygon is an inverse pyramid polygon and the top one is an inverse corner (but not pyramid) polygon. The generating function is

$$G_3(x, y) = 2y^2 \sum_{a,b,c,d=1}^{\infty} x^{2a-2d} (H_d - P_d) P_{b+c+d}. \tag{12}$$

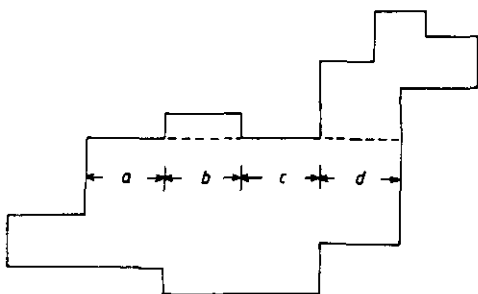


Figure 5. The fourth special case of polygons with concavity one where the top polygon is an inverse corner polygon (but not pyramid polygon) and the main polygon is a corner polygon.

Consider the fourth case as shown in figure 5 where the main polygon is a corner polygon and the top one is an inverse corner (but not pyramid) polygon. The generating function is

$$G_4(x, y) = 2y^2 \sum_{a=0}^{\infty} \sum_{b,c,d=1}^{\infty} x^{-2d} (H_d - P_d) H_{a+b+c+d}. \tag{13}$$

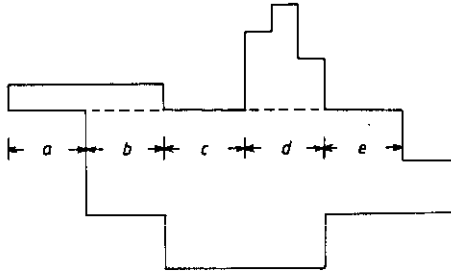


Figure 6. The fifth special case of polygons with concavity one where the top polygon is a pyramid polygon and the main polygon is a corner polygon.

Consider the fifth case as shown in figure 6 where the top polygon is a pyramid polygon (but not a $1 \times m$ rectangle) and the main polygon is a corner polygon. The generating function is

$$G_5(x, y) = 2y^2 \sum_{a,b,c,d=1}^{\infty} \sum_{e=0}^{\infty} x^{2a} (x^{-2d} P_d - y^2) H_{b+c+d+e}. \tag{14}$$

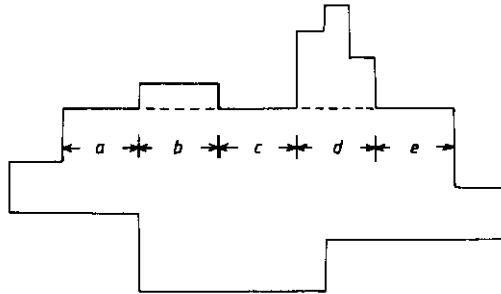


Figure 7. The sixth special case of polygons with concavity one where the top polygon is a pyramid polygon and the main polygon is a convex polygon.

Consider the sixth and final case as shown in figure 7 where the top polygon is a pyramid polygon and the main one is a convex polygon. The generating function is

$$G_6(x, y) = y^2 \sum_{a,e=0}^{\infty} \sum_{b,c,d=1}^{\infty} R_{a+b+c+d+e} (2x^{-2d} P_d - y^2). \tag{15}$$

We use the computer algebra program REDUCE to calculate the generating function and the final result is

$$\begin{aligned} G_t &= G_1 + G_2 + G_3 + G_4 + G_5 + G_6 \\ &= 4x^4y^2 A(x, y)/(1-x^2)\Delta^{5/2} + x^4y^2 B(x, y)/(1-x^2)[(1-x^2)^2 - y^2]\Delta^3 \\ &= x^6y^6 + 7x^8y^6 + 8x^6y^8 + 26x^{10}y^6 + 92x^8y^8 + 29x^6y^{10} + \dots \end{aligned} \tag{16}$$

where

$$\begin{aligned}
 A &= (1 - x^2)^5 - y^2(1 - x^2)^3(4 + 3x^2) + 6y^4(1 - x^2) - 2y^6(2 - x^2 + x^4) + y^8 \\
 B &= -4(1 - x^2)^8 + 8y^2(1 - x^2)^6(3 + 2x^2) - y^4(1 - x^2)^4(60 + 35x^2 + 10x^4 - x^6) \\
 &\quad + y^6(1 - x^2)^2(80 - 3x^2 + 28x^4 + 9x^6 - 2x^8) \\
 &\quad + 2y^8(-30 + 31x^2 - 13x^4 + 37x^6 + 7x^8) \\
 &\quad + 2y^{10}(12 - 5x^2 - 17x^4 - 23x^6 + x^8) - y^{12}(4 - 5x^2 - 24x^4 + x^6) - 3y^{14}x^2.
 \end{aligned}$$

When $x = y$ we have

$$\begin{aligned}
 G &= 4G_c = 16x^6A/(1 - x^2)(1 - 4x^2)^{5/2} + 4x^6B/(1 - x^2)(1 - 3x^2 + x^4)(1 - 4x^2)^3 \\
 &= \sum_n N_n x^n = 4x^{12} + 60x^{14} + 588x^{16} + 4636x^{18} + \dots + \dots + \dots
 \end{aligned} \tag{17}$$

where

$$\begin{aligned}
 A &= 1 - 9x^2 + 25x^4 - 23x^6 + 3x^8 \\
 B &= -4 + 56x^2 - 300x^4 + 773x^6 - 973x^8 + 535x^{10} - 90x^{12} + 24x^{14}.
 \end{aligned}$$

Expanding the generating function (17) about the singularity at $x^2 = \frac{1}{4}$, we obtain

$$G = (128)^{-1}(1 - 4x^2)^{-3} - 3(256)^{-1}(1 - 4x^2)^{-5/2} + O(1 - 4x^2)^{-2}. \tag{18}$$

It follows from the series expansions

$$\begin{aligned}
 (1 - 4x^2)^{-3} &= \sum_{m=0}^{\infty} (m + 1)(m + 2)2^{2m-1}x^{2m} \\
 (1 - 4x^2)^{-5/2} &= \sum_{m=0}^{\infty} (2m + 3)!x^{2m}/6(m + 1)!m!
 \end{aligned} \tag{19}$$

that

$$N_n = n^2 2^{n-10} [1 - 4(2/n\pi)^{1/2} + O(1/n)] \tag{20}$$

which confirms the conjecture (2) of Enting *et al* (1991) for $c = 1$.

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