Rigorous derivation of the perimeter generating function for the mean-squared radius of gyration of convex polygons

2010 J. Phys. A: Math. Theor. 43 265001

(http://iopscience.iop.org/1751-8121/43/26/265001)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **43** (2010) 265001 (7pp) doi:10.1088/1751-8113/43/26/265001

Rigorous derivation of the perimeter generating function for the mean-squared radius of gyration of convex polygons

Keh Ying Lin

Department of Physics, National Tsing Hua University, Hsinchu 300, Taiwan, Republic of China

E-mail: lin@phys.nthu.edu.tw

Received 21 December 2009
Published 2 June 2010
Online at stacks.iop.org/JPhysA/43/265001

Abstract

We have rigorously derived the perimeter generating function for the mean-squared radius of gyration of convex polygons. This function was first conjectured by Jensen. His nonrigorous result is based on the analysis of the long series expansions.

PACS numbers: 05.50.+q, 05.70.Jk, 02.10.Ox

Jensen [1] derived long series expansions for the perimeter generating functions of the radius of gyration of various self-avoiding polygons on the square lattice with a convexity constraint. He used the series to obtain six algebraic exact solutions for the generating functions. In the special cases of rectangular, Ferrers, pyramid and staircase polygons, the exact solutions are relatively simple and have been proved rigorously by Lin [2, 3]. Recently the exact solution for directed convex polygons was also verified by Lin [4]. We shall rigorously prove the last exact solution conjectured by Jensen for convex polygons in this paper.

The perimeter generating function for the number of self-avoiding polygons on the square lattice is given by

$$P(z) = \sum_{n=2}^{\infty} p_n z^{2n}, \tag{1}$$

where p_n is the number of self-avoiding polygons with perimeter $2n$. The anisotropic perimeter generating function for the number of polygons is defined by

$$P(x, y) = \sum_{r=1}^{\infty} \sum_{s=1}^{\infty} p_{r,s} x^{2r} y^{2s}, \tag{2}$$

where $p_{r,s}$ is the number of polygons with horizontal width r and vertical height s.

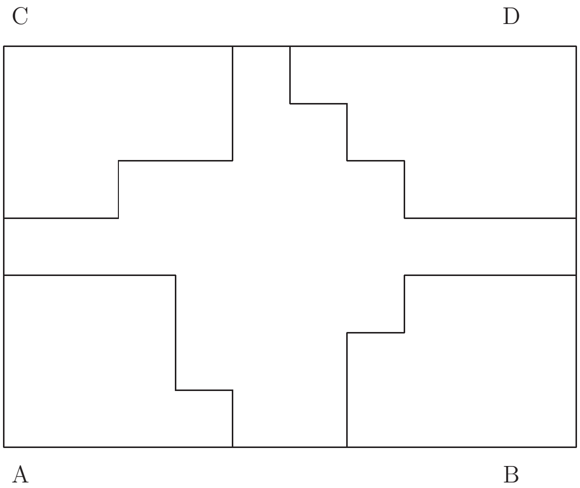

Figure 1. A convex polygon bounded by a rectangle. The rectangle is divided into five polygons where the middle one is a convex polygon and the others are Ferrers polygons.

The generating functions for the area-weighted moments of convex polygons on the square lattice are defined by

$$P^{(m)}(z) = \sum_n z^{2n}\left[\sum_k k^m c_{n,k}\right], \tag{3}$$

where $c_{n,k}$ is the number of polygons with $2n$ steps and area k. The corresponding anisotropic generating functions are

$$P^{(m)}(x, y) = \sum_{r,s} x^{2r} y^{2s}\left[\sum_k k^m c_{r,s,k}\right], \tag{4}$$

where $c_{r,s,k}$ is the number of polygons with width r, height s and area k. Our definition of $P^{(2)}$ is slightly different from Enting and Guttmann [5]. In their definition, k^2 is replaced by $k(k-1)/2$.

The perimeter generating function for the mean-squared radius of gyration of polygons is given by [1]

$$R(z) = \sum_{n=2}^{\infty} r_n z^{2n}, \tag{5}$$

where

$$\begin{aligned} r_n &= \sum_{\Omega_n} \sum_{i,j=0}^{2n-1} [(x_i - x_j)^2 + (y_i - y_j)^2]/2 \\ &= \sum_{\Omega_n}\left[2n\sum_{j=0}^{2n-1}\left(x_j^2 + y_j^2\right) - \left(\sum_{j=0}^{2n-1} x_j\right)^2 - \left(\sum_{j=0}^{2n-1} y_j\right)^2\right]; \end{aligned} \tag{6}$$

the symbol Ω_n means the set of all polygons of perimeter length $2n$, and the coordinate of each vertex j on the polygon is denoted by (x_j, y_j).

A convex polygon with $2n$ steps and area k is bounded by an $r \times s$ rectangle as shown in figure 1. The bounding rectangle is divided into five polygons, where the middle one is a convex polygon and the others are Ferrers polygons (denoted by A, B, C and D). For convenience, the area of the Ferrers polygon A is also denoted by A, etc.

The Ferrers polygon C as shown in figure 1 is formed from a directed walk with right or up steps, extended at the starting point with a horizontal step and at the end point with a vertical step, and then closed by straight lines to form a polygon. Each Ferrers polygon C is characterized by a set of integers $(a_1, b_m, \ldots, a_m, b_1)$ such that the directed walk starts with a_1 right steps, followed by b_m up steps, etc. We define

$$C^*(a, b) = a_1(b_1 + \cdots + b_m)^2 + a_2(b_1 + \cdots + b_{m-1})^2 + \cdots + a_m b_1^2 + b_1(a_1 + \cdots + a_m)^2 + b_2(a_1 + \cdots + a_{m-1})^2 + \cdots + b_m a_1^2. \tag{7}$$

For each convex polygon, it can be shown that [3]

$$2n \sum_{j=0}^{2n-1} \left(x_j^2 + y_j^2\right) - \left(\sum_{j=0}^{2n-1} x_j\right)^2 - \left(\sum_{j=0}^{2n-1} y_j\right)^2 = \sum_{m=1}^{5} g_m, \tag{8}$$

where

$$\begin{aligned} g_1 &= n^2(n^2 + 2)/3,\\ g_2 &= -2n^2(A + B + C + D),\\ g_3 &= 2(A + B + C + D)^2,\\ g_4 &= 2n(A^* + B^* + C^* + D^*),\\ g_5 &= -2[(A + B)^2 + (C + D)^2 + (A + C)^2 + (B + D)^2]. \end{aligned}$$

The contribution of g_m to the radius of gyration generating function is denoted by $R^{(m)}(z)$ and we have

$$R(z) = \sum_{j=1}^{5} R^{(j)}(z). \tag{9}$$

It follows from

$$\frac{z}{2}\frac{\mathrm{d}}{\mathrm{d}z} z^{2n} = n z^{2n} \tag{10}$$

that

$$R^{(1)}(z) = \sum_{n=2}^{\infty} [n^2(n^2 + 2)/3] p_n z^{2n} = \left[\frac{1}{3}\left(\frac{z}{2}\frac{\mathrm{d}}{\mathrm{d}z}\right)^4 + \frac{2}{3}\left(\frac{z}{2}\frac{\mathrm{d}}{\mathrm{d}z}\right)^2\right] P(z). \tag{11}$$

Similarly it follows from

$$A + B + C + D = rs - k \tag{12}$$

that

$$R^{(2)}(z) = -2\left(\frac{z}{2}\frac{\mathrm{d}}{\mathrm{d}z}\right)^2 \left[\frac{xy}{4}\frac{\partial^2}{\partial x \partial y} P(x, y)\right]_{x=y=z} + 2\left(\frac{z}{2}\frac{\mathrm{d}}{\mathrm{d}z}\right)^2 P^{(1)}(z). \tag{13}$$

It follows from

$$(A + B + C + D)^2 = r^2 s^2 - 2rsk + k^2 \tag{14}$$

that

$$R^{(3)}(z) = \left[2\left(\frac{x}{2}\frac{\partial}{\partial x}\right)^2 \left(\frac{y}{2}\frac{\partial}{\partial y}\right)^2 P(x, y) - 4\left(\frac{x}{2}\frac{\partial}{\partial x}\right)\left(\frac{y}{2}\frac{\partial}{\partial y}\right) P^{(1)}(x, y)\right]_{x=y=z} + 2P^{(2)}(z). \tag{15}$$

The perimeter generating function for convex polygons was first derived by Delest and Viennot [6] using the method of algebraic language, and later by several authors using different methods [7–9]:

$$P(z) = \frac{z^4(1-6z^2+11z^4-4z^6)}{(1-4z^2)^2} - \frac{4z^8}{(1-4z^2)^{3/2}}. \tag{16}$$

The corresponding anisotropic generating function was derived by Lin and Chang [9]:

$$P(x,y) = \frac{x^2y^2 f(x,y)}{\Delta^2} - \frac{4x^4y^4}{\Delta^{3/2}}, \tag{17}$$

where

$$f = 1 - 3(x^2+y^2) + 3x^4 + 3y^4 + 5x^2y^2 - (x^2+y^2)(x^4+y^4) - x^2y^2(x^2-y^2)^2,$$
$$\Delta = 1 - 2x^2 - 2y^2 + (x^2-y^2)^2.$$

Based on series expansions, Enting and Guttmann [5] obtained two generating functions for the area weighted moments of the number of convex polygons:

$$P^{(1)} = \frac{z^4(1-12z^2+50z^4-76z^6+42z^8-48z^{10}+32z^{12})}{(1-4z^2)^4} + \frac{4z^8}{(1-4z^2)^{5/2}}, \tag{18}$$

$$P^{(2)} = \frac{M}{(1-4z^2)^6} + \frac{N}{(1-4z^2)^{9/2}}, \tag{19}$$

where

$$\begin{aligned} M = {} & z^4 - 16z^6 + 172z^8 - 1116z^{10} + 4062z^{12} - 8304z^{14} \\ & + 10\,160z^{16} - 7872z^{18} + 3840z^{20} - 1024z^{22}, \end{aligned}$$
$$N = -54z^8 + 312z^{10} - 648z^{12} + 624z^{14} - 240z^{16}.$$

These conjectures were confirmed by Lin [10, 11] who also derived the anisotropic generation function

$$P^{(1)}(x,y) = \frac{x^2y^2T}{\Delta^4} + \frac{4x^4y^4[1-(x^2-y^2)^2]}{\Delta^{5/2}}, \tag{20}$$

where

$$\begin{aligned} T = {} & 1 - 6(x^2+y^2) + 15(x^4+y^4) + 20x^2y^2 - 20(x^6+y^6) - 18(x^4y^2+x^2y^4) \\ & + 15(x^8+y^8) - 8(x^6y^2+x^2y^6) + 28x^4y^4 - 6(x^{10}+y^{10}) \\ & + 22(x^8y^2+x^2y^8) - 40(x^6y^4+x^4y^6) + x^{12} + y^{12} - 12(x^{10}y^2+x^2y^{10}) \\ & - 5(x^8y^4+x^4y^8) + 64x^6y^6 + 2(x^{12}y^2+x^2y^{12}) + 18(x^{10}y^4+x^4y^{10}) \\ & - 20(x^8y^6+x^6y^8) + 2(x^{12}y^4+x^4y^{12}) - 8(x^{10}y^6+x^6y^{10}) + 12x^8y^8. \end{aligned}$$

Substituting the above expressions into equations (11), (13) and (15), we get

$$R^{(1)}(z) = \frac{2z^4F_1}{(1-4z^2)^6} + \frac{8z^8G_1}{(1-4z^2)^{11/2}}, \tag{21}$$

where

$$F_1 = 4 - 63z^2 + 696z^4 - 4022z^6 + 14\,160z^8 - 29\,824z^{10} + 34\,560z^{12} - 16\,896z^{14},$$
$$G_1 = -48 + 381z^2 - 1494z^4 + 2872z^6 - 2200z^8.$$

$$R^{(2)}(z) = \frac{32z^8F_2}{(1-4z^2)^6} + \frac{16z^8G_2}{(1-4z^2)^{11/2}}, \tag{22}$$

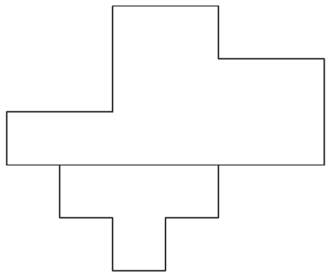

Figure 2. A convex polygon divided into a pyramid polygon on top of another upside-down pyramid polygon.

where

$$F_2 = -24 + 226z^2 - 1023z^4 + 2684z^6 - 4080z^8 + 3264z^{10} - 1024z^{12},$$
$$G_2 = 40 - 305z^2 + 1174z^4 - 2528z^6 + 2792z^8 - 1176z^{10}, \tag{23}$$
$$R^{(3)}(z) = \frac{4z^8 F_3}{(1-4z^2)^6} + \frac{4z^8 G_3}{(1-4z^2)^{11/2}},$$

where

$$F_3 = 77 - 810z^2 + 3772z^4 - 10\,072z^6 + 16\,132z^8 - 14\,988z^{10} + 6568z^{12} + 912z^{14} - 576z^{16},$$
$$G_3 = -75 + 648z^2 - 2528z^4 + 5584z^6 - 7240z^8 + 5120z^{10} - 1440z^{12}.$$

We define a generating function $R(K)$ which generates convex polygons with perimeter $2n$ and weight K. It follows from the rotational symmetry of square lattice that

$$R(A^*) = R(B^*) = R(C^*) = R(D^*) = R^{(6)}, \tag{24}$$
$$R[(A+B)^2] = R[(C+D)^2] = R[(A+C)^2] = R[(B+D)^2] = R^{(7)}. \tag{25}$$

Consequently, we have

$$R^{(4)} = 4z\frac{\partial}{\partial z}R^{(6)}, \tag{26}$$
$$R^{(5)} = -8R^{(7)}. \tag{27}$$

We use the method of Lin and Chang [9] to derive $R^{(6)}$ and $R^{(7)}$. Each convex polygon can be uniquely divided into a pyramid polygon on top of a directed convex polygon. There are three possibilities: pyramid polygon, a pyramid polygon on top of another upside-down pyramid polygon (see figure 2) and a pyramid polygon on top of a directed convex polygon (see figure 3). The perimeter generating function of convex polygons is [9]

$$P(x,y) = G(x,y) + \sum_{r=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} G_{r+m+n}(x,y)x^{-2m}G_m(x,y)$$
$$+2\sum_{r=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=0}^{\infty} G_{r+m}(x,y)x^{-2m}H_{m+n}(x,y), \tag{28}$$

where G is the generating function of pyramid polygons, G_m is the generating function of pyramid polygons with width m and H_m is the generating function of directed convex polygons whose width at top is m.

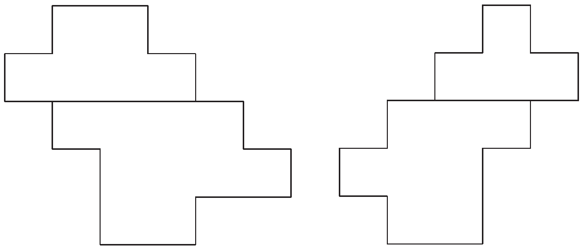

Figure 3. A convex polygon divided into a pyramid polygon on top of a directed convex polygon.

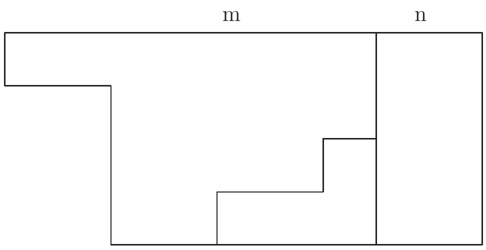

Figure 4. The upside-down pyramid polygon as shown in figure 2 has the width m. The convex polygon is bounded by a minimum rectangle and the distance between the upside-down pyramid polygon and the vertical boundary of the rectangle is denoted by n.

We use the method of Lin and Chang to calculate the contribution of each category of convex polygons to $R^{(6)} = R(B^*)$. The contribution of pyramid polygons is zero since $A^* = B^* = 0$. The contribution S_1 of convex polygons shown in figure 2 can be calculated as follows. Consider a convex polygon such that the upside-down pyramid has the width m, height h, weights b and b^* (figure 4). The weight B^* of the whole convex polygon (one pyramid polygon on top of an upside-down pyramid polygon) is

$$B^* = b^* + 2nb + n^2h + nh^2. \tag{29}$$

It follows from the above equation that

$$S_1 = \sum_{r=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} G_{r+m+n}(z)z^{-2m}\left[G_m^{(B^*)} + 2nG_m^{(B)} + n^2 D_y G_m + n D_y^2 G_m\right]_{x=y=z}, \tag{30}$$

where

$$D_y = \frac{y}{2}\frac{\partial}{\partial y}.$$

$G_m^{(B^*)}(z)$ and $G_m^{(B)}(z)$ generate pyramid polygons with perimeter $2n$ and weights B^* and B, respectively, such that the width of polygons is m.

Similarly the contribution of convex polygons shown in figure 3 is

$$S_2 = \sum_{r=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=0}^{\infty} G_{r+m}(z)z^{-2m}H_{m+n}^{(B^*)}(z) + \sum_{r=0}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} G_{m+n}(z)z^{-2m}\left[H_{r+m}^{(B^*)} + 2nH_{r+m}^{(B)} + n^2 D_y H_{r+m} + n D_y^2 H_{r+m}\right]_{x=y=z}. \tag{31}$$

The generating functions $G_m^{(B)}$, $G_m^{(B^*)}$, $H_m^{(A^*)}$, $H_m^{(B)}$ and $H_m^{(B^*)}$ have been calculated by Lin [11] recently. We use *Mathmatica* to carry out calculation and the results are

$$R^{(6)} = S_1 + S_2 = \frac{2z^8(6 - 42z^2 + 115z^4 - 174z^6 + 144z^8 - 32z^{10})}{(1 - 4z^2)^5} + \frac{2z^8(-5 + 24z^2 - 46z^4 + 56z^6 - 24z^8)}{(1 - 4z^2)^{9/2}} \tag{32}$$

and

$$R^{(4)}(z) = 4z\frac{\mathrm{d}}{\mathrm{d}z}R^{(6)} = \frac{16z^8(24 - 186z^2 + 690z^4 - 1678z^6 + 2544z^8 - 2016z^{10} + 512z^{12})}{\Delta^6} + \frac{16z^8(-20 + 110z^2 - 324z^4 + 668z^6 - 752z^8 + 336z^{10})}{\Delta^{11/2}}.$$

The generating function $R[(A + B)^2] = R^{(7)}$ can be derived in a similar way and the result is

$$R^{(5)}(z) = -8R^{(7)} = \frac{16z^8 F_5}{\Delta^6} + \frac{16z^8 G_5}{\Delta^{11/2}}, \tag{33}$$

$$F_5 = -20 + 210z^2 - 973z^4 + 2575z^6 - 4077z^8 + 3795z^{10} - 1706x^{12} - 228x^{14} + 144z^{16},$$
$$G_5 = 19 - 163z^2 + 631z^4 - 1388z^6 + 1800z^8 - 1304z^{10} + 360z^{12},$$

$$R(z) = \sum_{j=1}^{5} R^{(j)}(z) = \frac{2z^4(1 - 2z^2)(4 - 55z^2 + 388z^4 - 1058z^6 + 956z^8 + 2064x^{10} - 6592z^{12} + 6400z^{14})}{(1 - 4z^2)^6} - \frac{4z^8(15 + 22z^2 - 408z^4 + 1664z^6 - 3720z^8 + 3456z^{10})}{(1 - 4z^2)^{11/2}}, \tag{34}$$

which was first conjectured by Jensen [1].

References

[1] Jensen I 2005 Perimeter generating functions for the mean-squared radius of gyration of convex polygons *J. Phys. A: Math. Gen.* **38** L769–75

[2] Lin K Y 2006 Rigorous derivation of the perimeter generating functions for the mean-squared radius of gyration of rectangular, Ferrers and pyramid polygons *J. Phys. A: Math. Gen.* **39** 8741–5

[3] Lin K Y 2007 Rigorous derivation of the radius of gyration generating function for staircase polygons *J. Phys. A: Math. Theor.* **40** 1419–26

[4] Lin K Y 2009 Rigorous derivation of the radius of gyration generating functions for directed convex polygons *Chin. J. Phys. (Taipei)* **47** 578–612

[5] Enting I G and Guttmann A J 1989 Area-weighted moments of convex polygons on the square lattice *J. Phys. A: Math. Gen.* **22** 2639–42

[6] Delest M P and Viennot G 1984 Algebraic languages and polyominoes enumeration *Theor. Comput. Sci.* **34** 169–208

[7] Guttmann A J and Enting I G 1988 The number of convex polygons on the square and honeycomb lattices *J. Phys. A: Math. Gen.* **21** 467–74

[8] Kim D 1988 The number of convex polyominoes with given perimeter *Discrete Math.* **70** 47–51

[9] Lin K Y and Chang S J 1988 Rigorous results for the number of convex polygons on the square and honeycomb lattices *J. Phys. A: Math. Gen.* **21** 2635–42

[10] Lin K Y 1989 Rigorous result for the area-weighted moments of convex polygons on the square lattice *J. Phys. A: Math. Gen.* **22** 4263–9

[11] Lin K Y 1989 Rigorous result for the area-weighted moments of convex polygons on the square lattice *Chin. J. Phys. (Taipei)* **27** 399–424