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2007 J. Phys. A: Math. Theor. 40 1419

(http://iopscience.iop.org/1751-8121/40/6/N01)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **40** (2007) 1419–1426 doi:10.1088/1751-8113/40/6/N01

COMMENT

Rigorous derivation of the radius of gyration generating function for staircase polygons

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Received 1 October 2006, in final form 29 December 2006
Published 23 January 2007
Online at stacks.iop.org/JPhysA/40/1419

Abstract
We have rigorously derived the perimeter-generating function for the mean-squared radius of gyration of staircase polygons. This function was first obtained 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

In a recent letter, 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 and pyramid polygons, the exact solutions are relatively simple and have been proved rigorously by Lin [2]. We shall rigorously derive the generating function for the mean-squared radius of gyration of staircase polygons.

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

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

where p_n is the number of self-avoiding polygons with perimeter $2n$. The perimeter-generating function for mean-squared radius of gyration of polygons is given by [1]

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

where

$$r_n = \sum_{\Omega_n} \sum_{i,j=0}^{2n-1} [(x_i - x_j)^2 + (y_i - y_j)^2]/2$$
$$= \sum_{\Omega_n} \left[2n \sum_{j=0}^{2n-1} \left(x_j^2 + y_j^2\right) - \left(\sum_{j=0}^{2n-1} x_j\right)^2 - \left(\sum_{j=0}^{2n-1} y_j\right)^2 \right], \qquad (3)$$

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

The staircase polygon was first studied by Pólya [3] who showed for $n > 1$ that

$$p_n = \frac{(2n!)}{(4n-2)n!^2}. \qquad (4)$$

Consequently, the perimeter-generating function is

$$P(z) = (1 - 2z - \sqrt{1-4z})/2. \qquad (5)$$

The anisotropic staircase polygon was studied by Lin *et al* [4] and the corresponding perimeter-generating function is

$$P(x, y) = \sum_{r=1}^{\infty} \sum_{s=1}^{\infty} p_{r,s} x^r y^s = \left[1 - x - y - \sqrt{(1-x-y)^2 - 4xy}\,\right]\big/2, \qquad (6)$$

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

The staircase polygons with $2n$ steps are formed from a directed walk as follows. The directed walk starts from the origin with a_1 right steps, followed by b_1 up steps and so on until $a_1 + b_1 + \cdots + a_i + b_i = n$. Then, the walk returns to the origin with c_1 left steps, followed by d_1 down steps and so on until $c_1 + d_1 + \cdots + c_j + d_j = n$. We have [2]

$$2n \sum_{j=0}^{2n-1} \left(x_j^2 + y_j^2\right) - \left(\sum_{j=0}^{2n-1} x_j\right)^2 - \left(\sum_{j=0}^{2n-1} y_j\right)^2 = \sum_{m=1}^{9} g_m \qquad (7)$$

where

$$g_1 = n^2(n^2+2)/3 \qquad g_2 = -2n^2[A(a,b) + A(c,d)]$$
$$g_3 = 2[A(a,b) + A(c,d)]^2 \qquad g_4 = -4[A(a,b)]^2$$
$$g_5 = -4[A(c,d)]^2 \qquad g_6 = 2nB(a,b)$$
$$g_7 = 2nB(c,d) \qquad g_8 = 2nC(a,b)$$
$$g_9 = 2nC(c,d)$$

and $A(a, b)$, $B(a, b)$ and $C(a, b)$ are defined by

$$A(a_1, b_1) = B(a_1, b_1) = C(a_1, b_1) = 0 \qquad (8)$$
$$A(a,b) = a_i(b_1 + \cdots + b_{i-1}) + a_{i-1}(b_1 + \cdots + b_{i-2}) + \cdots + a_2 b_1 \qquad (9)$$
$$B(a,b) = a_i(b_1 + \cdots + b_{i-1})^2 + a_{i-1}(b_1 + \cdots + b_{i-2})^2 + \cdots + a_2 b_1^2 \qquad (10)$$
$$C(a,b) = b_1(a_2 + \cdots + a_i)^2 + b_2(a_3 + \cdots + a_i)^2 + \cdots + b_{i-1} a_i^2. \qquad (11)$$

The contribution of g_m to the radius of gyration generating function is denoted by $R_m(z)$ and we have

$$R(z) = \sum_{m=1}^{9} R_m(z), \qquad (12)$$

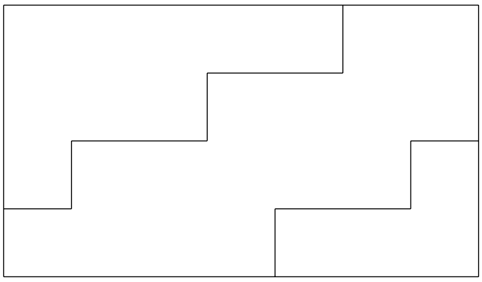

Figure 1. A staircase polygon with $2n$ steps and area k is bounded by an $r \times s$ rectangle.

where

$$R_1(z) = \sum_{n=2}^{\infty} [n^2(n^2+2)/3] p_n z^n = \left[\frac{1}{3} \left(z\frac{\mathrm{d}}{\mathrm{d}z} \right)^4 + \frac{2}{3} \left(z\frac{\mathrm{d}}{\mathrm{d}z} \right)^2 \right] P(z)$$
$$= \frac{z(1-6z+24z^2-24z^3)}{(1-4z)^{7/2}} - z. \tag{13}$$

We have

$$R_4(z) = R_5(z) \qquad R_6(z) = R_7(z) = R_8(z) = R_9(z) \tag{14}$$

directly from rotation and reflection symmetries of the staircase polygons.

A staircase 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 three polygons. It follows from the definition of A that the area of the polygon located in the upper-left corner is $A(c, d)$ and the area of the polygon in the lower-right corner is $A(a, b)$. We have

$$A(a, b) + A(c, d) = rs - k. \tag{15}$$

Enting and Guttmann [5] considered two generating functions for the area-weighted moments of the number of convex polygons on the square lattice:

$$P_1(z) = \sum_n z^n \left[\sum_k k c_{n,k} \right] \qquad P_2(z) = \sum_n z^n \sum_k [k(k-1)/2] c_{n,k}, \tag{16}$$

where $c_{n,k}$ is the number of polygons with $2n$ steps and area k. Based on the series expansions, they nonrigorously obtained these two generating functions. Their results are confirmed rigorously by Lin [6, 7]. We use the methods of Lin [8] and Temperley [9] to obtain the following generating functions for the area-weighted moments of the number of staircase polygons:

$$P_1(z) = \sum_n z^n \left[\sum_k k c_{n,k} \right] = \frac{z^2}{1-4z} \tag{17}$$

$$P_1(x, y) = \sum_{r,s} x^r y^s \left[\sum_k k c_{r,s,k} \right] = \frac{xy}{(1-x-y)^2 - 4xy} \tag{18}$$

$$P_2(z) = \sum_n z^n \left[\sum_k k^2 c_{n,k} \right] = \frac{z^2(1-2z+2z^2)}{(1-4z)^{5/2}} \tag{19}$$

where $c_{r,s,k}$ is the number of staircase polygons with width r, height s and area k. The generating functions P_1 and P_2 can also be computed from the functional equations, which the perimeter and area generating functions satisfy [10, 11].

It follows from equation (15) that

$$\begin{aligned} R_2(z) &= -2\left(z\frac{\mathrm{d}}{\mathrm{d}z}\right)^2\left[xy\frac{\partial^2}{\partial x\partial y}P(x,y)\right]_{x=y=z} + 2\left(z\frac{\mathrm{d}}{\mathrm{d}z}\right)^2 P_1(z) \\ &= -\frac{8z^2(1-5z+16z^2-18z^3)}{(1-4z)^{7/2}} + \frac{8z^2(1-3z+4z^2)}{(1-4z)^3} \end{aligned} \tag{20}$$

where $P(x,y)$ is defined by (6). It follows from

$$[A(a,b)+A(c,d)]^2 = r^2s^2 - 2rsk + k^2 \tag{21}$$

that

$$\begin{aligned} R_3(z) &= \left[2\left(x\frac{\partial}{\partial x}\right)^2\left(y\frac{\partial}{\partial y}\right)^2 P(x,y) - 4\left(x\frac{\partial}{\partial x}\right)\left(y\frac{\partial}{\partial y}\right)P_1(x,y)\right]_{x=y=z} + 2P_2(z) \\ &= \frac{4z^2(1-6z+17z^2-24z^3+12z^4)}{(1-4z)^{7/2}} + \frac{4z^2(-1+4z-10z^2+8z^3)}{(1-4z)^3}. \end{aligned} \tag{22}$$

We define three generating functions

$$G_1(x,y) = \sum_{r,s} x^r y^s \left[\sum_A A c_{r,s,A}\right] \tag{23}$$

$$G_2(z) = \sum_n z^n \left[\sum_B B c_{n,B}\right] \tag{24}$$

$$G_3(z) = \sum_n z^n \left[\sum_A A^2 c_{n,A}\right] \tag{25}$$

where $c_{r,s,A}$ is the number of staircase polygons with width r, height s and A; $c_{n,A}$ is the number of staircase polygons with perimeter $2n$ and A; A and B are defined by (9) and (10). It follows from equation (15) that

$$\begin{aligned} G_1(x,y) &= \left[xy\frac{\partial^2}{\partial x\partial y}P(x,y) - P_1(x,y)\right]\Big/2 \\ &= \frac{xy(1-x-y)}{2[1-2x-2y+(x-y)^2]^{3/2}} - \frac{xy}{2[1-2x-2y+(x-y)^2]}. \end{aligned} \tag{26}$$

It is well known that the Temperley method [9] can be applied for classes of column-convex polygons in order to obtain explicit expressions for generating functions with respect to counting parameters such as perimeter, height, width, last column height and area [12]. We shall use the methods of Lin [8] and Temperley [9] to derive the generating functions G_2 and G_3.

The generating function $P(x,y)$ for the isotropic staircase polygons can be written in the form

$$P(x,y) = \sum_{m=1}^{\infty} S_m(x,y) \tag{27}$$

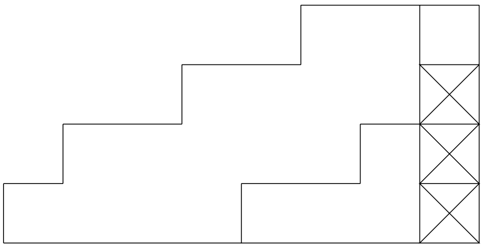

Figure 2. When one unit square is placed near the upper-right corner of a staircase polygon with height s, the area of A is increased by $s-1$ as shown by three unit squares with cross.

where S_m is the generating function corresponding to all polygons whose width at the top is m. It can be shown [4] that

$$S_{m+1} = xS_m + y\sum_{n=0}^{\infty} S_{m+n+1} \tag{28}$$

where $S_0 = y$. It follows from equation (28) that

$$S_{m+1} = (1+x-y)S_m - xS_{m-1} \tag{29}$$

and the solution of this recursion relation is [4]

$$S_m = yu^m \tag{30}$$

where

$$u = \left[1+x-y-\sqrt{(1-x-y)^2-4xy}\,\right]/2 \tag{31}$$

is a root of the equation

$$u^2 - (1+x-y)u + x = 0. \tag{32}$$

The generating function $G_1(x, y)$ can also be written in the form [6]

$$G_1(x, y) = \sum_{m=1}^{\infty} S'_m(x, y) \tag{33}$$

where

$$S'_{m+1} = xS'_m + y\sum_{n=0}^{\infty} S'_{m+n+1} + x\left[y\frac{\partial}{\partial y} - 1\right]S_m. \tag{34}$$

The last term in equation (34) is explained as follows. Consider a staircase polygon with height s whose top row width is m. If we put one unit square to the upper-right corner as shown in figure 2, then the area of A is increased by $s-1$.

It follows from equations (30) and (34) that

$$\begin{aligned} S'_{m+1} - (1+x-y)S'_m + xS'_{m-1} &= x\left[y\frac{\partial}{\partial y} - 1\right](S_m - S_{m-1}) \\ &= \frac{xy^2[mu^m - (m-1)u^{m-1}]}{[1-2x-2y+(x-y)^2]^{1/2}} \end{aligned} \tag{35}$$

and the solution is

$$S'_m = [am(m-1)/2 + bm]u^m \tag{36}$$

where

$$a = \frac{y^2\left[1 - x - y + \sqrt{1 - 2x - 2y + (x - y)^2}\,\right]}{2[1 - 2x - 2y + (x - y)^2]}$$

$$b = \frac{xy^2\left[1 - x + y - \sqrt{1 - 2x - 2y + (x - y)^2}\,\right]}{2[1 - 2x - 2y + (x - y)^2]^{3/2}}.$$

The generating function $G_2(z)$ can be written in the form

$$G_2(z) = \sum_{m=1}^{\infty} H_m(z) \tag{37}$$

where

$$H_{m+1}(z) = zH_m(z) + z\sum_{n=0}^{\infty} H_{m+n+1}(z) + \Delta_m(z) \tag{38}$$

$$\Delta_m(z) = \left[x\left(y\frac{\partial}{\partial y} - 1\right)^2 S_m(x, y)\right]_{x=y=z}$$

$$= \left[\frac{m^2z^4}{1 - 4z} + \frac{mz^3(1 - 3z)}{(1 - 4z)^{3/2}}\right]w^m \tag{39}$$

$$w = \frac{1 - \sqrt{1 - 4z}}{2}. \tag{40}$$

The last term in equation (38) follows from the fact that when we put one unit square to the upper-right corner of the staircase polygon as shown in figure 2, then the value of B is increased by $(s - 1)^2$. The solution of the recursion relation

$$H_{m+1} - H_m + zH_{m-1} = \Delta_m - \Delta_{m-1} \tag{41}$$

is

$$H_m = [a'm(m - 1)(m - 2)/6 + b'm(m - 1)/2 + c'm]w^m \tag{42}$$

where

$$a' = \frac{z^3(1 - 2z)}{(1 - 4z)^{3/2}} + \frac{z^3}{1 - 4z}$$

$$b' = \frac{z^2(1 - 2z - 4z^2)}{2(1 - 4z)^{3/2}} + \frac{z^2(1 - 2z)^2}{2(1 - 4z)^2}$$

$$c' = \frac{z^2(-2 + 5z - z^2)}{2(1 - 4z)^{3/2}} + \frac{z^2(-2 + 8z - 9z^2)}{2(1 - 4z)^2}.$$

The generating function G_2 can be derived from

$$H_2 - wH_1 = (b' + c')w^2 = z(1 - w)G_2 + \Delta_1 \tag{43}$$

and the result is

$$G_2(z) = \frac{z^2(1 - 2z)^2}{2(1 - 4z)^{5/2}} - \frac{z^2(1 - 2z)}{2(1 - 4z)^2}. \tag{44}$$

The generating function $G_3(z)$ can be written in the form

$$G_3(z) = \sum_{m=1}^{\infty} S''_m(z). \tag{45}$$

It follows from

$$(A + s - 1)^2 = A^2 + 2A(s - 1) + (s - 1)^2 \tag{46}$$

that

$$S''_{m+1}(z) = zS''_m(z) + z\sum_{n=0}^{\infty} S''_{m+n+1}(z) + \Delta'_m(z) + \Delta_m(z) \tag{47}$$

$$\Delta'_m(z) = \left[2x\left(y\frac{\partial}{\partial y} - 1\right)S'_m(x, y)\right]_{x=y=z}. \tag{48}$$

The recursion relation is

$$S''_{m+1} - S''_m + zS''_{m-1} = \Delta'_m - \Delta'_{m-1} + \Delta_m - \Delta_{m-1} \tag{49}$$

whose solution is

$$S''_m = [a''m(m-1)(m-2)(m-3)/24 + b''m(m-1)(m-2)/6 + c''m(m-1)/2 + d''m]w^m \tag{50}$$

where

$$a'' = \frac{3z^3(1-2z)}{(1-4z)^{3/2}} + \frac{3z^3(1-4z+2z^2)}{(1-4z)^2}$$
$$b'' = \frac{z^2(1-4z-3z^2+21z^3)}{(1-4z)^{5/2}} + \frac{z^2(1-2z-5z^2+9z^3)}{(1-4z)^2}$$
$$c'' = \frac{z^2(1-6z+18z^2-8z^3)}{2(1-4z)^{5/2}} + \frac{z^2(1-8z+18z^2+12z^3-12z^4)}{2(1-4z)^3}$$
$$d'' = \frac{z^2(-2+21z-79z^2+66z^3+30z^4)}{2(1-4z)^{7/2}} + \frac{z^2(-2+16z-35z^2+24z^3+6z^4)}{2(1-4z)^3}.$$

The generating function G_3 can be derived from

$$S''_2 - wS''_1 = (c'' + d'')w^2 = z(1-w)G_3 + \Delta_1 + \Delta'_1 \tag{51}$$

and the result is

$$G_3(z) = \frac{z^2(1-6z+18z^2-28z^3+12z^4)}{2(1-4z)^{7/2}} - \frac{z^2(1-4z+10z^2-8z^3)}{2(1-4z)^3}. \tag{52}$$

We have

$$R_4(z) = -4G_3(z) \tag{53}$$

$$R_6(z) = 2z\frac{\mathrm{d}}{\mathrm{d}z}G_2(z) = \frac{2z^2(1-5z+12z^2-12z^3)}{(1-4z)^{7/2}} - \frac{2z^2(1-3z+4z^2)}{(1-4z)^3}, \tag{54}$$

and the final result is

$$\begin{aligned} R(z) &= R_1(z) + R_2(z) + R_3(z) + 2R_4(z) + 4R_6(z) \\ &= \frac{z(1-6z+24z^2-60z^3+64z^4)}{(1-4z)^{7/2}} - z, \end{aligned} \tag{55}$$

which was derived by Jensen nonrigorously [1].

The methods of Temperley [9] and Lin [8] can be applied to derive the remaining two generating functions conjectured by Jensen for the directed convex and convex polygons. It is possible to treat higher moments of the radius of gyration by similar methods.

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