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COMMENT

Rigorous derivation of the perimeter generating functions for the mean-squared radius of gyration of rectangular, Ferrers and pyramid polygons

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Abstract
We have derived rigorously the perimeter generating functions for the mean-squared radius of gyration of rectangular, Ferrers and pyramid polygons. These functions were found by Jensen recently. His nonrigorous results are based on the analysis of the long series expansions.

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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 find 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 can easily be proved rigorously. I shall comment on the difficulty to derive rigorously the other three exact solutions at the end of this comment.

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

$$P(z) = \sum_n p_{2n} z^n, \tag{1}$$

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

$$R(z) = \sum_n r_{2n} z^n, \tag{2}$$

where

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

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

A rectangular polygon is characterized by width a and height b. The perimeter generating function for the number of rectangular polygons is

$$P(z) = \sum_{a=1}^{\infty} \sum_{b=1}^{\infty} z^a z^b = z^2/(1-z)^2. \tag{4}$$

The radius of gyration generation function is

$$R(z) = \sum_{a=1}^{\infty} \sum_{b=1}^{\infty} r_{a,b} z^a z^b, \tag{5}$$

where $r_{a,b}$ sums over all vertices of one rectangular polygon of width a and height b. Using the identity

$$1^2 + 2^2 + \cdots + n^2 = n(n+1)(2n+1)/6, \tag{6}$$

we obtain the following expression:

$$r_{a,b} = n^2(n^2+2)/3, \tag{7}$$

where $n = a + b$. Using the following identities where $f_k(z) = \sum_{m=1}^{\infty} m^k z^m$:

$$f_1 = z/(1-z)^2, \tag{8}$$

$$f_2 = z(1+z)/(1-z)^3, \tag{9}$$

$$f_3 = z(1+4z+z^2)/(1-z)^4, \tag{10}$$

$$f_4 = z(1+11z+11z^2+z^3)/(1-z)^5, \tag{11}$$

$$f_5 = z(1+26z+66z^2+26z^3+z^4)/(1-z)^6, \tag{12}$$

we obtain

$$R(z) = \sum_{n=2}^{\infty} n^2(n^2+2)(n-1)z^n/3 = 2z^2(1+z)^2(4+z)/(1-z)^6, \tag{13}$$

which was first derived nonrigorously by Jensen.

The Ferrers polygons [1] with $2n$ steps are formed from a directed walk with $n-2$ 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. The generating function is

$$P(z) = \sum_{n=2}^{\infty} 2^{n-2} z^n = z^2/(1-2z). \tag{14}$$

The directed walk starts from the origin with a_1 horizontal steps, then followed by b_1 vertical steps, and so on. Each Ferrers polygon is characterized by a set of integers

$(a_1, b_1, \ldots, a_m, b_m)$ where $a_1 + b_1 + \cdots + a_m + b_m = n$. Therefore the generation function can also be derived in the following way:

$$P(z) = \sum_{a=1}^{\infty}\sum_{b=1}^{\infty} z^{a+b} + \cdots + \sum_{a_1,b_1,\ldots,a_m,b_m} z^{a_1+b_1+,,+a_m+b_m} + \cdots$$
$$= z^2/(1-z)^2 + \cdots + z^{2m}/(1-z)^{2m} + \cdots = z^2/(1-2z). \quad (15)$$

The corresponding radius of gyration generation function is

$$R(z) = \sum_{m=1}^{\infty} R_m(z), \quad (16)$$

where

$$R_m(z) = \sum_{a_1,b_1,\ldots,a_m,b_m} r_{a_1,b_1,\ldots,a_m,b_m} z^{a_1+b_1+,,+a_m+b_m}. \quad (17)$$

After a straightforward calculation, we find

$$r_{a_1,b_1,\ldots,a_m,b_m} = n^2(n^2+2)/3 + \Delta(a_1, b_1, \ldots, a_m, b_m), \quad (18)$$

where

$$\Delta(a_1, b_1) = 0,$$
$$\Delta(a_1, b_1, a_2, b_2) = -2a_2b_1(n-a_2)(n-b_1),$$
$$\Delta(a_1, b_1, \ldots, a_m, b_m) = -2n^2A - 2A^2 + 2n(B+C),$$
$$A = b_1(a_2 + \cdots + a_m) + b_2(a_3 + \cdots + a_m) + \cdots + b_{m-1}a_m,$$
$$B = b_1(a_2 + \cdots + a_m)^2 + b_2(a_3 + \cdots + a_m)^2 + \cdots + b_{m-1}a_m^2,$$
$$C = a_m(b_1 + \cdots + b_{m-1})^2 + a_{m-1}(b_1 + \cdots + b_{m-2})^2 + \cdots + a_2b_1^2.$$

Substituting equation (18) into equation (16), we obtain

$$R(z) = R_0 + \sum_{m=2}^{\infty} D_m(z), \quad (19)$$

where

$$R_0(z) = \sum_{n=2}^{\infty} \frac{n^2(n^2+2)}{3} 2^{n-2} z^n = \frac{2z^2}{(1-2z)^5}(4 - 7z + 22z^2 - 20z^3 + 8z^4), \quad (20)$$

$$D_2(z) = -4f_1^4 - 12 f_2 f_1^2 f_0 - 2 f_2^2 f_0^2, \quad (21)$$

$$D_m(z) = \sum_{a_1,b_1,\ldots,a_m,b_m} \Delta(a_1, b_1, \ldots, a_m, b_m) z^{a_1+b_1+\cdots+a_m+b_m}$$
$$= -\frac{m(m-1)}{6}(11m^2 - 15m - 2) f_1^4 f_0^{2m-4}$$
$$-\frac{2}{3}m(m-1)(5m-1) f_2 f_1^2 f_0^{2m-3} - m(m-1) f_2^2 f_0^{2m-2}. \quad (22)$$

The radius of gyration generating function is

$$R(z) = \frac{2z^2}{(1-2z)^5}(4 - 7z + 13z^2 - 10z^3 + 2z^4), \quad (23)$$

which was first derived by Jensen nonrigorously [1].

A pyramid (stack) polygon of $(m+1)$ layers is characterized by $(w, a_1, \ldots, a_m, b_1, \ldots, b_m)$. The top layer is a $w \times 1$ rectangle, the layer below is an $(a_1 + w + b_1) \times 1$ rectangle, and so on. The perimeter length is $2n$ where

$$n = w + a_1 + \cdots + a_m + b_1 + \cdots + b_m + m + 1. \tag{24}$$

The perimeter generating function of pyramid polygons is [2]

$$\begin{aligned} P(z) &= \left(\sum_{w=1}^{\infty} z^{w+1}\right)\left(1 + \sum_{m=1}^{\infty}\sum_{a_j=0}^{\infty}\sum_{b_j=0}^{\infty} z^{a_1+\cdots+a_m+b_1+\cdots+b_m+m}\right) \\ &= \frac{z^2}{1-z}\sum_{m=0}^{\infty}\frac{z^m}{(1-z)^{2m}} = \frac{z^2(1-z)}{1-3z+z^2}. \end{aligned} \tag{25}$$

The radius of gyration generating function of pyramid polygons is

$$\begin{aligned} R(z) &= \sum_{n=2}^{\infty}\frac{n^2(n^2+2)}{3}z^n \\ &\quad + \sum_{w=1}^{\infty}\sum_{m=1}^{\infty}\sum_{a_j=0}^{\infty}\sum_{b_j=0}^{\infty} r(w, a_1, \ldots, a_m, b_1, \ldots, b_m) z^{w+a_1+\cdots+a_m+b_1+\cdots+b_m+m+1}. \end{aligned} \tag{26}$$

We find

$$r(w, a_1, \ldots, a_m, b_1, \ldots, b_m) = n^2(n^2+2)/3 + \Delta(w, a_1, \ldots, a_m, b_1, \ldots, b_m), \tag{27}$$

where

$$\begin{aligned} &\Delta(w, a_1, b_1) = -2(n-1)[a_1(n-a_1) + b_1(n-b_1)], \\ &\Delta(w, a_1, \ldots, a_m, b_1, \ldots, b_m) = -2n^2A - 2B + 2nC, \\ &A = (a_1 + 2a_2 + \cdots + ma_m) + (b_1 + 2b_2 + \cdots + mb_m), \\ &B = (a_1 + 2a_2 + \cdots + ma_m)^2 + (b_1 + 2b_2 + \cdots + mb_m)^2, \\ &C = (a_1 + 2^2a_2 + \cdots + m^2a_m) + (b_1 + 2^2b_2 + \cdots + m^2b_m) \\ &\qquad + (a_1 + a_2 + \cdots + a_m)^2 + (a_2 + \cdots + a_m)^2 + \cdots + a_m^2 \\ &\qquad + (b_1 + b_2 + \cdots + b_m)^2 + (b_2 + \cdots + b_m)^2 + \cdots + b_m^2. \end{aligned}$$

Substituting equation (27) into equation (26), we obtain

$$R(z) = R_0 + \sum_{m=1}^{\infty} D_m(z), \tag{28}$$

where

$$\begin{aligned} R_0(z) &= \sum_{w=1}^{\infty}\sum_{m=0}^{\infty}\sum_{a_j=0}^{\infty}\sum_{b_j=0}^{\infty}\frac{n^2(n^2+2)}{3}z^n \\ &= \left[\frac{1}{3}\left(z\frac{\mathrm{d}}{\mathrm{d}z}\right)^4 + \frac{2}{3}\left(z\frac{d}{dz}\right)^2\right]\frac{z^2(1-z)}{1-3z+z^2} \\ &= \frac{8z^2 - 54z^3 + 250z^4 - 645z^5 + 929z^6 - 722z^7 + 301z^8 - 100z^9 + 15z^{10} - z^{11}}{(1-3z+z^2)^5} \end{aligned} \tag{29}$$

$$D_1(z) = -z^2\big(8f_2f_1 + 12f_1^2 + 8f_2f_0 + 8f_1f_0\big)\big/(1-z) - z^2\big(8f_2f_1f_0 + 8f_1^3 + 12f_1^2f_0\big), \tag{30}$$

$$D_m(z) = \sum_{w,a_1,b_1,\ldots,a_m,b_m} \Delta(w,a_1,\ldots,a_m,b_1,\ldots,b_m) z^{w+a_1+b_1+\cdots+a_m+b_m+m+1}$$
$$= -\frac{\left[2f_1^2(4m+5)+12f_1f_2+2f_0f_1(m+1)(m+2)+6f_0f_2(m+1)\right]m(m+1)z^{m+1}}{3(1-z)^{2m-1}}$$
$$-\frac{\left[4f_1^3(5m-2)+f_0f_1^2(15m^2+11m-8)+4f_0f_1f_2(4m-1)\right]m(m+1)z^{m+1}}{3(1-z)^{2m-2}}$$
$$-\frac{4f_0f_1^3m(m^2-1)(4m-1)z^{m+1}}{3(1-z)^{2m-3}}. \quad (31)$$

After a long calculation, the final result is

$$R(z) = \frac{8z^2-54z^3+214z^4-489z^5+605z^6-386z^7+177z^8-120z^9+19z^{10}-z^{11}}{(1-3z+z^2)^5}, \quad (32)$$

which was found by Jensen [1].

The perimeter and radius of gyration generating functions for the rectangular, Ferrers, and pyramid polygons can be rigorously derived easily because all these functions can be expressed as summations of infinite series such that each term of the series is defined explicitly. An example is given by equation (26). The situation is very different for the staircase, directed convex and convex polygons. To derive rigorously the perimeter generating functions for these polygons, the first step is to obtain recursion relations and find their solutions [2, 3]. However, the corresponding recursion relations for the radius of gyration generating functions are very complicated and the traditional method [4] to solve such relations does not work.

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