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2005 J. Phys. A: Math. Gen. 38 L769

(http://iopscience.iop.org/0305-4470/38/46/L01)

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

J. Phys. A: Math. Gen. **38** (2005) L769–L775 doi:10.1088/0305-4470/38/46/L01

LETTER TO THE EDITOR

Perimeter generating functions for the mean-squared radius of gyration of convex polygons

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Received 15 September 2005
Published 2 November 2005
Online at stacks.iop.org/JPhysA/38/L769

Abstract
We have derived long series expansions for the perimeter generating functions of the radius of gyration of various polygons with a convexity constraint. Using the series we numerically find simple (algebraic) exact solutions for the generating functions. In all cases the size exponent $\nu = 1$.

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

1. Introduction

A well-known long standing problem in combinatorics and statistical mechanics is to find the generating function for self-avoiding polygons (or walks) on a two-dimensional lattice. The models are of tremendous inherent interest as well as serving as simple models of polymers and vesicles [1–3]. Despite strenuous effort over the past 50 years or so, this problem has not been solved on any regular two-dimensional lattice. However, there are many simplifications of this problem that are solvable [4], but all the simpler models impose an effective directedness or other constraint that reduces the problem, in essence, to a one-dimensional problem.

One particular class of exactly solved polygon models are those with a convexity constraint (see figure 1). On the square lattice a polygon is said to be *convex* if it is convex with respect to both vertical and horizontal lines, i.e., any vertical line will intersect the polygon at zero or two horizontal edges while similarly any horizontal line will intersect the polygon at zero or two vertical edges. Alternatively, a convex polygon is a SAP of a length equal to the perimeter of its minimal bounding rectangle. If we further demand that the polygon must include the vertices in some of the corners of the minimal bounding rectangle, we can define a further five polygon models as illustrated in figure 1. The full perimeter and area generating functions are known for all these models [4]. Also of great interest is the mean-square radius of gyration, $\langle R^2 \rangle_n$, which measures the typical size of a polygon with perimeter n. In this letter, we report on work leading to conjectured exact solutions for the generating functions associated with the mean-square radius of gyration for the class of convex polygons.

An *n-step self-avoiding walk* $\boldsymbol{\omega}$ is a sequence of *distinct* vertices $\omega_0, \omega_1, \ldots, \omega_n$ such that each vertex is a nearest neighbour of it predecessor. SAWs are considered distinct up to translations of the starting point ω_0. A self-avoiding polygon of length n is an $n-1$-step SAW such that ω_0 and ω_{n-1} are nearest neighbours and a closed loop can be formed by inserting a single additional step joining the two end points. We shall use the symbol $\boldsymbol{\Omega}_n$ to mean the set of all SAPs of perimeter length n. Generally SAPs are considered distinct up to a translation, so if there are p_n SAPs of length n there are $2np_n$ walks (the factor of 2 arising since the walk can go in two directions). One expects in general that $p_n \sim A\mu^n n^{\alpha-3}$, where μ is the so-called connective constant while α is a critical exponent. In our cases μ and α are known from the exact solutions for the perimeter generating functions

$$\mathcal{P}(x) = \sum_n p_{2n} x^n \sim A(x)(1 - \mu^2 x)^{2-\alpha}, \tag{1}$$

where we took into account that polygons on the square lattice have even length. The generating functions thus have a singularity at the critical point $x_c = 1/\mu^2$ with critical exponent $2 - \alpha$. The function $A(x)$ is analytic at $x = x_c$. Note that both μ and α are model dependent.

The mean-square radius of gyration of n-step polygons is defined by

$$\langle R^2 \rangle_n = \frac{1}{2n^2 p_n} \sum_{\Omega_n} \sum_{i,j=0}^{n-1} (\omega_i - \omega_j)^2, \tag{2}$$

where we expect that $\langle R^2 \rangle_n \sim Bn^{2\nu}$. It is advantageous to look at the quantity $r_n = n^2 p_n \langle R^2 \rangle_n$, which is an integer, and in particular we shall study the associated generating function

$$\mathcal{R}(x) = \sum_n r_{2n} x^n \sim B(x)(1 - \mu^2 x)^{-(\alpha+2\nu)}, \tag{3}$$

where we again used that r_n is non-zero only when n is even.

The values for the critical exponents are known exactly, though non-rigorously, for self-avoiding polygons due to the work by Nienhuis [5], $\alpha = 1/2$ and $\nu = 3/4$. As we shall demonstrate later, the exponent α takes on several different values for the convex polygons studied in this letter, but the exponent $\nu = 1$ in all cases.

In the next section, we briefly describe the algorithm used to calculate r_n and in the following section we list the various perimeter generating functions.

2. Computer enumeration

The first terms in the series for the polygon generating function are calculated using transfer matrix techniques to count the number of polygons spanning rectangles $W + 1$ edges wide and $L + 1$ edges long. The transfer matrix technique involves drawing a line through the rectangle intersecting a set of edges. For each configuration of occupied or empty edges along the intersection, we maintain a (perimeter) generating function for partial polygons cutting the intersection in that particular pattern. Due to the convexity constraint a vertical line will intersect the polygon exactly twice. The upper edge of the convex polygon performs a directed walk taking steps to the right and up until it reaches the top of the rectangle where it turns and then performs a directed walk with steps to the right and down. Likewise the lower edge performs a directed walk with right and down steps until it hits the bottom of the rectangle where it turns and takes only right and up steps. A convex polygon is formed once the two walks meet. In order to specify a configuration we just need to know the positions of the edges and whether or not the top and bottom of the rectangle have been touched. All the possible configurations can then be encoded by four $(W + 1) \times (W + 1)$-matrices, one matrix for each possibility of touched borders. As the vertical boundary line is moved one step forward, the

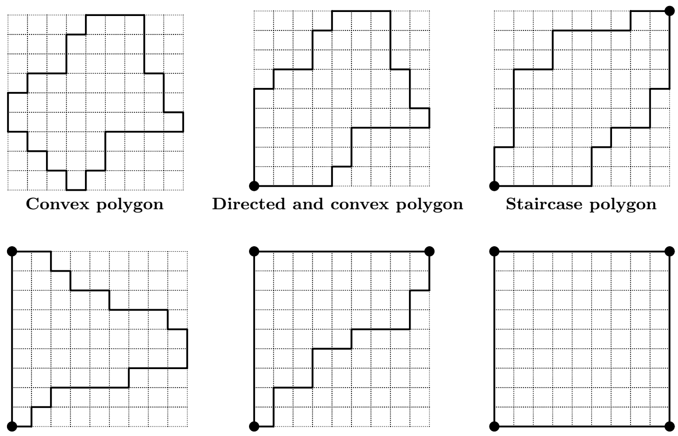

Figure 1. Examples of the types of convex polygons we consider in this letter.

matrices are updated to allow for all the legal moves of the edge-walks (the walks must be directed as described above and never cross). The updating involves simple double sums over the indices. This approach was used by Guttmann and Enting [6] and is very efficient. However, in one iteration many steps can be inserted and this makes the calculation of the contributions to the radius of gyration somewhat cumbersome. We find it more convenient to use an algorithm in which the convex polygons in a given rectangle are enumerated by moving the intersection so as to add one vertex at a time. The method we used to enumerate convex polygons on the square lattice is a specialization of the method originally devised by Enting [7] for the enumeration of self-avoiding polygons. As noted earlier, convex polygons can be viewed as SAPs with a number of steps equal to the perimeter of the minimal bounding rectangle. So we could simply take our previous algorithm [8, 9], which we generalized in order to calculate the radius of gyration, and only extract the terms counting convex polygons. Due to the convexity constraint we were able to simplify the algorithm somewhat and make it more efficient. However, the algorithm is still quite similar to the SAP enumeration algorithm so we would not describe it further. Suffice to say that the method for calculating the radius of gyration coefficients r_n has been described in [9].

Using this algorithm we quickly (a few hours of CPU time) calculated the radius of gyration of the polygon models of figure 1 to length $n = 110$, giving us 56 terms in the half-perimeter series. The first few terms p_n and r_n are listed in table 1. The full series for the generating functions studied in this letter can be obtained by sending a request to the author or via the web at http://www.ms.unimelb.edu.au/˜iwan/.

3. The exact generating functions

In this section we use the series for r_n to find (numerically) the exact perimeter generating functions for the radius of gyration of convex polygons.

The perimeter generating function for convex polygons was first obtained by Delest and Viennot [10] using the method of algebraic languages and later by several other authors using different methods [6, 11, 12]:

$$\mathcal{P}_{\text{Convex}}(x) = \frac{x^2 - 6x^3 + 11x^4 - 4x^5}{(1-4x)^2} - \frac{4x^4}{(1-4x)^{3/2}}. \tag{4}$$

Table 1. The number of polygons p_n and their mean-squared radius of gyration $r_n = n^2 p_n \langle R^2 \rangle_n$.

	Convex polygons		Directed and convex polygons		Staircase polygons	
n	p_n	r_n	p_n	r_n	p_n	r_n
4	1	8	1	8	1	8
6	2	66	2	66	2	66
8	7	600	6	522	5	444
10	28	5 164	20	3 772	14	2 710
12	120	41 768	70	25 138	42	15 512
14	528	317 584	252	157 212	132	84 756
16	2 344	2 280 792	924	935 140	429	446 952
18	10 416	15 573 120	3 432	5 343 160	1 430	2 291 718
20	46 160	101 743 312	12 870	29 541 450	4 862	11 485 760
22	203 680	639 664 960	48 620	158 920 172	16 796	56 486 716
24	894 312	3 889 101 336	184 756	835 390 460	58 786	273 405 288
26	3 907 056	22 961 959 168	705 432	4 305 416 136	208 012	1 305 401 916
28	16 986 352	132 118 984 560	2 704 156	21 812 985 652	742 900	6 159 651 344
30	73 512 288	743 046 249 664	10 400 600	108 875 244 952	2 674 440	28 766 573 800
32	316 786 960	4 095 077 270 128	40 116 600	536 326 527 048	9 694 845	133 128 274 320
34	1 359 763 168	22 163 717 040 384	155 117 520	2 611 304 032 624	35 357 670	611 143 639 110
36	5 815 457 184	118 021 533 366 432	601 080 390	12 582 098 181 466	129 644 790	2 785 335 811 920
38	24 788 842 304	619 313 064 407 680	2 333 606 220	60 058 408 242 252	477 638 700	12 612 104 460 780
40	105 340 982 248	3 206 924 122 635 928	9 075 135 300	284 257 070 075 212	1 767 263 190	56 773 091 159 400
	Stack polygons		Ferrers diagrams		Rectangular polygons	
4	1	8	1	8	1	8
6	2	66	2	66	2	66
8	5	444	4	366	3	288
10	13	2 541	8	1 640	4	900
12	34	12 840	16	6 404	5	2 280
14	89	59 113	32	22 696	6	4 998
16	233	253 600	64	74 832	7	9 856
18	610	1 029 802	128	233 312	8	17 928
20	1 597	4 002 112	256	695 680	9	30 600
22	4 181	15 005 189	512	2 000 128	10	49 610
24	10 946	54 603 436	1 024	5 578 752	11	77 088
26	28 657	193 743 969	2 048	15 166 464	12	115 596
28	75 025	672 725 072	4 096	40 336 384	13	168 168
30	196 418	2 292 470 170	8 192	105 256 960	14	238 350
32	514 229	7 685 026 612	16 384	270 135 296	15	330 240
34	1 346 269	25 392 243 845	32 768	683 188 224	16	448 528
36	3 524 578	82 826 447 752	65 536	1 705 443 328	17	598 536
38	9 227 465	267 077 278 409	131 072	4 207 935 488	18	786 258
40	24 157 817	852 322 922 488	262 144	10 274 078 720	19	1 018 400

From this we see that the critical point $x_c = 1/4$ (and thus $\mu = 2$) while the critical exponent $2 - \alpha = -2$ (and thus $\alpha = 4$), corresponding to the dominant double pole at $x = x_c$. In addition there is a sub-dominant square root correction. Informed by this result it is natural to assume that the generation function for the mean-squared radius of gyration has a similar form. That is we assume that $\mathcal{R}(x) = [A(x) + B(x)\sqrt{1-4x}]/(1-4x)^{\gamma}$, where $A(x)$ and $B(x)$ are polynomials. Using the method of differential approximants [13] we easily established that $\gamma = 6$. Next we wrote a simple Maple routine to find such a solution, that is we solve for the unknown coefficients a_i and b_i of $A(x)$ and $B(x)$. We simply form the series expansion for $[A(x) + B(x)\sqrt{1-4x}]$, match the series coefficients to those of $\mathcal{R}(x)(1-4x)^6$ and solve the resulting set of linear equations in the coefficients a_i and b_i. In this fashion we found a solution with polynomials of degree 10 requiring not more than 22 unknown coefficients. Since we have more than 50 known terms r_{2n} there are at least 30 unused series coefficients which serve as strong checks on the correctness of our solution. The generating function for the mean-squared radius of gyration of convex polygons is

$$\mathcal{R}_{\text{Convex}}(x) = \frac{2x^2(1-2x)(4-55x+388x^2-1058x^3+956x^4+2064x^5-6592x^6+6400x^7)}{(1-4x)^6} - \frac{4x^4(15+22x-408x^2+1664x^3-3720x^4+3456x^5)}{(1-4x)^{11/2}}. \tag{5}$$

From this we see that the critical exponent $\alpha + 2\nu = 6$ and thus $\nu = 1$. This should be compared to the result for self-avoiding polygons $\nu = 3/4$ [5]. Physically, there is a simple argument for $\nu = 1$. Convex polygons are relevant to the description of vesicles in the *inflated* regime, where they are space filling, and since the radius of gyration measures a typical size of a polygon $\langle R^2\rangle_n$ is proportional to a typical area and hence $\nu = 1$ for convex polygons. The value $\nu = 3/4$ means that SAPs are much more ramified.

Directed and convex polygons were considered by Lin and Chang [11]. They calculated the full anisotropic generating function for directed and convex polygons. In the isotropic case which we consider here their result reduces to the very simple form

$$\mathcal{P}_{\text{DirConv}}(x) = \frac{x^2}{(1-4x)^{1/2}}, \tag{6}$$

so we have $x_c = 1/4$ while $2 - \alpha = -1/2$ and thus $\alpha = 5/2$. As for the convex case we start by looking for a solution to $\mathcal{R}(x)$ of the same form, that is $\mathcal{R}(x) = A(x)/(1-4x)^{\gamma}$, with $\gamma = 9/2$ determined from differential approximants. However we were not successful at first, so next we tried a solution of the same form as for convex polygons and found that

$$\mathcal{R}_{\text{DirConv}}(x) = \frac{-x^2+20x^3-48x^4+24x^5-168x^6+384x^7}{(1-4x)^{9/2}} + \frac{9x^2-44x^3+72x^4-32x^5}{(1-4x)^3}. \tag{7}$$

So in this case we find the critical exponent $\alpha + 2\nu = 9/2$ and thus as before $\nu = 1$.

The model of staircase polygons is very well known and much studied, dating back at least to the work by Pólya [14] who showed that $p_{2n} = \frac{1}{4n-2}\binom{2n}{n}$ for $n \geqslant 2$. This result was obtained by Delest and Viennot [10] in the more elegant form $p_{2n+2} = C_n = \frac{1}{n+1}\binom{2n}{n}$, where C_n are the famous and ubiquitous Catalan numbers. Consequently the generating function is

$$\mathcal{P}_{\text{Stair}}(x) = (1 - 2x - \sqrt{1-4x})/2, \tag{8}$$

and $x_c = 1/4$, while $2 - \alpha = 1/2$ and thus $\alpha = 3/2$. As per the previous cases we quite readily find the radius of gyration generation function

$$\mathcal{R}_{\text{Stair}}(x) = \frac{x(1-6x+24x^2-60x^3+64x^4)}{(1-4x)^{7/2}} - x, \tag{9}$$

and we see that $\alpha + 2\nu = 7/2$ and once again $\nu = 1$.

Stack polygons were also considered by Lin and Chang [11] and their result for the generating function is

$$\mathcal{P}_{\text{Stack}}(x) = \frac{x^2(1-x)}{(1-3x+x^2)}. \tag{10}$$

The critical point is now given by the zero of $1 - 3x + x^2$ namely $x_c = 0.381\,966\,011\ldots$ and the critical exponent is $2 - \alpha = -1$ or $\alpha = 3$. In this case the radius of gyration generation function is of the same form and again we have $\nu = 1$. Explicitly we find that

$$\mathcal{R}_{\text{Stack}}(x) = \frac{8x^2 - 54x^3 + 214x^4 - 489x^5 + 605x^6 - 386x^7 + 177x^8 - 120x^9 + 19x^{10} - x^{11}}{(1 - 3x + x^2)^5}. \tag{11}$$

The generating function for Ferrers diagrams is trivial in that these polygons are simply 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 with $2n$ steps. It immediately follows that the generating function is

$$\mathcal{P}_{\text{Ferrers}}(x) = \frac{x^2}{(1 - 2x)}, \tag{12}$$

and we have $x_c = 2$ and $\alpha = 3$. The radius of gyration generation function is of the same form and with $\nu = 1$,

$$\mathcal{R}_{\text{Ferrers}}(x) = \frac{2x^2(4 - 7x + 13x^2 - 10x^3 + 2x^4)}{(1 - 2x)^5}. \tag{13}$$

Rectangular polygons are obviously the simplest case and the generating function is simply

$$\mathcal{P}_{\text{Rect}}(x) = \frac{x^2}{(1 - x)^2}, \tag{14}$$

so that $x_c = 1$ and $\alpha = 4$. The radius of gyration generating function is found to be

$$\mathcal{R}_{\text{Rect}}(x) = \frac{2x^2(1 + x)^2(4 + x)}{(1 - x)^6}, \tag{15}$$

and again we have $\nu = 1$.

Now that these results for the radius of gyration of convex polygons are known from the numerical work presented here it should be easier to prove them rigorously.

Acknowledgment

We gratefully acknowledge financial support from the Australian Research Council.

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