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On the Area of Square Lattice Polygons

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We consider the generating function of self-avoiding square lattice polygons grouped by both area and perimeter. The generating function for polygons of area n is found to diverge at $x_c = 0.251834$, with an exponent of zero. The mean perimeter of polygons with area n is found to be proportional to n, while the mean area of polygons with perimeter n is found to be proportional to $n^{1.5}$.

KEY WORDS: Square lattice polygons.

1. INTRODUCTION

The method of exact series expansions was refined and developed into a valuable tool by Domb and co-workers at Kings' College, London. For many problems, it remains the most powerful method of approximation. With the development of very fast computers, and the parallel development of algorithm refinement, it is now possible to make exact conjectures of critical exponents in favorable circumstances. The following study utilizes developments in computing hardware, algorithms, and analysis methods that have taken place over the last decade, and allows us to confidently conjecture certain critical exponents.

For many years the problem of self-avoiding polygons has been studied by calculating the terms in the generating function for polygons with given perimeter. This generating function, when twice differentiated, gives the "specific heat" of the N-vector model in the $N \to 0$ limit. Recently we were able to obtain[(1)] polygons to 56 steps on the square lattice and[(2)] 82 steps on the honeycomb lattice. An alternative problem, the behavior of the generating function of polygons by enclosed area, has received far less

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attention. In 1961 Hiley and Sykes[3] considered the distribution of polygons on the square and triangular lattices by both area and perimeter, obtaining data for all polygons up to perimeter 18 (square) and 16 (triangular) steps. The triangular data were sufficiently good to permit them to estimate the increase of mean area $\langle a_n \rangle$ of polygons with perimeter n, and they found $\langle a_n \rangle \sim n^{1.5 \pm 0.04}$. Many years later, Leibler *et al.*[4] gave heuristic arguments as to why the exponent should be 2ν, where $\nu = 3/4$ for the two-dimensional self-avoiding walk (SAW) problem.[5]

To define the problems more precisely, let p_n denote the number of polygons with perimeter n and generating function $P(x)$. Let a_n denote the number of polygons with area n and generating function $A(y)$. Let $\langle p_n \rangle$ denote the mean perimeter of all polygons with area n and generating function $\Lambda(y)$, and let $\langle a_n \rangle$ denote the mean area of all polygons with perimeter n and generating function $\Omega(x)$.

These quantities can all be derived from the generating function $\mathbf{P}(x, y)$,

$$\mathbf{P}(x, y) = \sum_n \sum_m p_{n,m} x^m y^n \tag{1}$$

where $p_{n,m}$ is the number of polygons with area n and perimeter m. Thus,

$$P(x) = \mathbf{P}(x, 1), \qquad A(y) = \mathbf{P}(1, y)$$

$$\langle p_n \rangle = \sum_m m \cdot p_{n,m} \Big/ \sum_m p_{n,m}, \qquad \langle a_m \rangle = \sum_n n \cdot p_{n,m} \Big/ \sum_n p_{n,m}$$

where the denominators of $\langle p_n \rangle$ and $\langle a_m \rangle$ can be written a_n and p_m, respectively. Further, for any finite n or m, the other sum in (1) is also finite. That is to say, $\mathbf{P}(x, y)$ can be expressed as a single sum in n or m with $p_{n,m}$ replaced by a polynomial in x or y, respectively. We wish to determine the singular behavior of the three generating functions $A(y)$, $\Lambda(y)$, and $\Omega(x)$. The generating function $P(x)$ has been discussed previously.[1,2]

In the fields of combinatorial mathematics and computer science, the same problems involving a subset of self-avoiding polygons, *convex* polygons, have been discussed for many years. Consider polygons on the square lattice. Then *row-convex* polygons are defined as those polygons (we dispense with the universal adjective self-avoiding) in which any vertical line on the dual lattice intersects either zero or two horizontal bonds of the convex polygon. Similarly, for *column-convex* polygons, any horizontal line on the dual lattice intersects either zero or two vertical bonds of the convex polygons. Polygons which are both row-convex and column-convex we denote simply as *convex*.

For row- (or equivalently column-) convex polygons, Temperley[6] and subsequently Polya[7] showed that the generating function of such polygons grouped by area takes a particularly simple form,

$$A(y) = y(1-y)^3/(1-5y+7y^2-4y^3)$$

which has a simple pole at 0.311957055..., whereas[7] the generating function for row-convex polygons, with respect to a diagonal line, grouped by perimeter has coefficients equal to $\binom{2n}{n}/(4n-2)$, so that the generating function has a cusplike square-root singularity with a "critical point" at $x_c = 1/4$.

For convex polygons, the generating function of polygons grouped by area has been studied by Klarner and Rivest[8] and subsequently by Bender.[9] They found that the generating function $A(y)$ is singular at $y_c = 0.433061923$, again with a simple pole, though a closed-form expression has never been found. For convex polygons grouped by perimeter, the generating function was first found by Delest and Viennot,[10] who showed that

$$P(x) = x^2[(1-6x+11x^2-4x^3)/(1-4x)^2 - 4x^2/(1-4x)^{3/2}]$$

which has a double pole at $x_c = 1/4$. This result was subsequently independently discovered by a number of authors.[11–13]

Thus we see from the simpler problems of convex and row-convex polygons that both the "critical points" and exponents are quite different for the two generating functions $A(y)$ and $P(x)$.

In the remainder of this paper we study these and related quantities for unrestricted self-avoiding polygons on the square lattice. Known results to date on some aspects of this problem are

$$P(x) \sim A(1-\mu x)^{1.5} + B$$

where $\mu = 2+\sqrt{2}$ (honeycomb), 6.958880 (square),[3] 4.15075 (triangular), and

$$\Omega(x) \sim C(1-x)^{-2.5} + D$$

The results for the exponent of $P(x)$ follow from Nienhuis' exact results[5] and scaling laws, and have been verified by series work of Guttmann and Enting[1,2] based on series of length 82, 56, and 25 terms for the honeycomb, square, and triangular[4] lattices, respectively. The series work

[3] For the square and honeycomb lattices only polygons with an even number of bonds are embeddable. Thus, the connective constant is the square of the SAW connective constant.

[4] The extension of the triangular lattice polygon series by the present authors has not yet been published.

cited also gave the quoted connective constants. The exponent for the generating function $\Omega(x)$ of mean areas was first given in ref. 3. Based on our enumerations, which are complete for polygons with perimeter up to 42 steps and area 20 (assuming a square lattice of unit lattice spacing), we conjecture that

$$A(x) \sim G + H \cdot \log(1 - \kappa x) \qquad \text{(square)}$$

where $\kappa = 3.97087...$ and the singularity may be some more complicated function of a logarithm. If we assume that the exponent is exactly $0_{\log}$, then we conjecture the following exact exponents:

$$a_n \sim \kappa^n \cdot n^{-1}, \qquad p_n \sim \mu^n \cdot n^{-5/2}$$

Analysis of the mean area series for square lattice polygons suggested $\langle a_n \rangle \sim n^{1.5}$, in agreement with the earlier estimate[5] of the exponent 1.50 ± 0.04. Analysis of the mean perimeter data gave $\langle p_n \rangle \sim n$, where the exponent is found to be 1.000 ± 0.003. This supports a conjecture of Whittington (unpublished) that the exponent is exactly 1.

In the next section we discuss the derivation of the series, and in Section 3 we present the analysis of the data.

2. ENUMERATION OF POLYGONS BY AREA AND PERIMETER

The series that we have calculated is the set of p_{nm}, the number of self-avoiding polygons of perimeter m and area n on the square lattice [1]. Our computational technique is a direct generalisation of the approach of Enting.[14] We obtain a truncated approximation to $\mathbf{P}(x, y)$ as

$$\mathbf{P}(x, y) \cong \sum_{m,n} a_{mn} G_{mn}(x, y) \tag{2}$$

where the sum is over the range defined by $1 \leqslant m \leqslant n$ and $m + n \leqslant 2W + 1$. Here $G_{mn}(x, y)$ is the generating function for all self-avoiding polygons that fit into a rectangle m steps wide and n steps long, but not into any rectangle less than n steps long. W is the maximum width, $W = \max(m)$, for which the G_{mn} are required. If the a_{mn} are obtained using the rules given in ref. 14, then the approximation (2) will give the coefficients p_{nm} correctly for $m \leqslant 4W + 2$. We have used $W = 10$ and so have enumerated polygons of up to 42 steps, with the additional y dependence giving the distribution according to area.

The combinatorics of combining the partial generating functions G_{mn} is exactly the same as specified in ref. 14. The calculation of the various

$G_{mn}(x, y)$ is a relatively simple generalization of our earlier procedure, which, in the present notation, determined $G_{mn}(x, 1)$.

The enumeration proceeds by building up a finite rectangular lattice, one site at a time, starting from the top left, building a column of sites downward and then building up successive columns one site at a time from the top down. As each site is added we have to consider all possible ways in which bonds leaving the site downward or to the right can be added. When considering the number of ways a bond can occur in a partly constructed polygon, we have to consider not only the presence or absence of a bond, but also the connectivity of bonds that are present. This is done[14] by labeling bonds with a 1 or 2, depending on whether the bond is at the top or bottom of a loop running through the partly constructed lattice. The number of ways of adding the two new bonds leaving a new site has to be considered in conjunction with the number of ways in which all other sites in the partly constructed lattice can be linked to sites that are yet to be added. The number of combinations grows rapidly. It is bounded above by 3^{W+2}; a generating function for the precise numbers of combinations is given in ref. 1, Eq. (10). These numbers define the size of vectors required in the construction of the G_{mn}. For $W = 10$ we require vectors with 15,511 components. The vector components combine partial generating functions (series in x and y) describing the number of ways of having sets of self-avoiding loops reaching the growing edge of the partly constructed rectangle in a specified manner. Each time a new site is added and the state of two new bonds is assigned, a factor of x^0, x^1, or x^2 is included in the partial generating function, depending on whether 0, 1, or 2 of the bonds were occupied (i.e., in states 1 or 2). A factor of y^0 or y^1 is included, depending on whether or not the square to the top left of the new site is outside or inside the polygon. For each possible combination of intersections of loops with the growing edge of the lattice we can determine whether a square is inside or outside any polygon that can be formed from the partly constructed loops by noting whether the number of bonds between the site and the top of the lattice is odd or even.

In summary, the new factors required when generalizing the method[14] to obtain the p_{mn} are the use of two-variable series throughout, the inclusion of the factors y^0 or y^1 when building up a new vector of loop generating functions, and a procedure for counting number of bonds to determine whether the factor should be y^0 or y^1. The requirement for series in two variables restricted us to $W \leqslant 10$, so that our series for p_{nm} can only be complete for $m \leqslant 42$. The coefficients p_{nm} are zero if $2n + 2 < m$ (or $n > m^2/16$). Thus, completeness for $m \leqslant 42$ implies completeness for $n \leqslant 20$. In practice we truncated the expansion at $m = 48$ and $n = 50$. Thus, for fixed $n \leqslant 20$, all nonzero p_{nm} are obtained correctly ($n = 13$–49 for $m = 28$) with the limit being set by the order q at which we truncated the series.

Table I. Coefficients p_{nm} of the Generating Function $P(x, y)$[a]

m	1	2	3	4	5	6	7	8	9	10	11	12
4	1											
6		2										
8			6	1								
10				18	8	2						
12					55	40	22	6	1			
14						174	168	134	72	30	8	2
16							566	676	656	482	310	151
18								1868	2672	2992	2592	2086
20									6237	10376	13160	12862
22										21050	39824	56162
24											71666	151878
26												245696
28												

m	13	14	15	16	17	18
16	68	22	6	1		
18	1392	864	456	218	88	30
20	11717	9332	7032	4748	3010	1728
22	61032	60864	54032	45936	35952	26858
24	234520	279492	301802	290754	268056	231156
26	576656	965136	1246080	1443896	1493528	1467628
28	847317	2181496	3928732	5448780	6720262	7404092
30		2937116	8229160	15850366	23468968	30631444
32			10226574	30974700	63482128	99831330
34				35746292	116385088	252724778
36					125380257	436678520
38						441125966

m	19	20	$A(y)$ Series	$\langle p_n \rangle$	$\langle a_n \rangle$
4			1	4	1
6			2	6	2
8			6	8	3.1428571429
10			19	9.89473684	4.4285714286
12			63	11.7460317	5.8548387097
14			216	13.5925926	7.4013605442
16			756	15.4391534	9.0585432267
18	8	2	2684	17.2831595	10.820277705
20	914	426	9638	19.1276198	12.681445995
22	18744	12456	34930	20.9736044	14.63708594
24	191910	151097	127560	22.820947	16.682878073
26	1356960	1212736	468837	24.6694779	18.815033267
28	7696852	7531072	1732702	26.5190437	21.030199678
30	35700744	39048104	6434322	28.3694636	23.325383019
32	137311068	168434122	23993874	30.2205738	25.697887518
34	420247680	607002280	89805691	32.072244	28.145271227
36	1001011854	1753545206	337237337	33.9243709	30.665308851
38	1636472360	3947661088	1270123530	35.7768731	33.255961787
40	1556301578	6126647748	4796310672	37.6296864	35.915353517
42		18155586993	18155586993	39.4827603	38.641749316

[a] The coefficient $p_{n,m}$ is the number of polygons with perimeter m and area n. The last three columns give, in order, the coefficients of the generating function of the area grouping $A(y)$, the mean perimeters for fixed area, and the mean area for fixed perimeter.

In Table I we show the coefficients p_{nm}, $n \leqslant 20$, $m \leqslant 42$, as well as the coefficients of the generating function $A(y)$ and the mean perimeters of polygons of area n, $\langle p_n \rangle$, and the mean areas of polygon of perimeter n, $\langle a_n \rangle$.

3. SERIES ANALYSIS

The series expansion of $A(y)$ is given up to the coefficient of y^{20} in Table I. We have analyzed the series by both ratio methods and the

Table II. Neville–Aitken Extrapolation of the Ratios and Unbiased Exponent Estimates of the Generating Function $A(y)$, the Number of Polygons Grouped by Area[a]

n	$e(n, 1)$	$e(n, 2)$	$e(n, 3)$	$e(n, 4)$	$e(n, 5)$
			Extrapolate ratios		
7	3.55026	3.85185	3.83862	3.87408	4.10248
8	3.59091	3.87542	3.94613	4.12530	4.37652
9	3.62420	3.89049	3.94323	3.93744	3.70262
10	3.65188	3.90099	3.94298	3.94240	3.94983
11	3.67542	3.91090	3.95553	3.98898	4.07050
12	3.69575	3.91928	3.96118	3.97812	3.95641
13	3.71346	3.92606	3.96332	3.97046	3.95323
14	3.72904	3.93163	3.96504	3.97134	3.97353
15	3.74286	3.93626	3.96639	3.97181	3.97311
16	3.75519	3.94014	3.96725	3.97095	3.96838
17	3.76626	3.94340	3.96787	3.97079	3.97027
18	3.77626	3.94617	3.96837	3.97082	3.97092
19	3.78532	3.94855	3.96875	3.97081	3.97078
			Extrapolate unbiased exponent estimates		
7	0.45192	0.49679	0.30467	−1.59668	−5.34879
8	0.41268	0.13802	−0.93832	−3.00998	−4.42329
9	0.38397	0.15427	0.21118	2.51018	9.41039
10	0.36141	0.15834	0.17460	0.08926	−3.54212
11	0.33767	0.10032	−0.16080	−1.05519	−3.05799
12	0.31557	0.07248	−0.06671	0.21554	2.75700
13	0.29605	0.06173	0.00264	0.23384	0.27501
14	0.27863	0.05223	−0.00480	−0.03210	−0.69694
15	0.26299	0.04407	−0.00897	−0.02565	−0.00791
16	0.24897	0.03866	0.00079	0.04307	0.24922
17	0.23635	0.03445	0.00285	0.01247	−0.08698
18	0.22494	0.03091	0.00262	0.00144	−0.03716
19	0.21457	0.02795	0.00279	0.00372	0.01227

[a] The left-hand column indexes the nonzero coefficients. Thus, the area is $n+1$ for entries in row n.

method of differential approximants.[15] The series was found to be very well behaved, with the various sequences studied by the ratio method being smoothly extrapolable by Neville–Aitken extrapolation, after some initial variations in the ratios of the early terms. Beyond 12 or 13 terms, stability was quite apparent. This, however, demonstrates the importance of obtaining series of sufficient length for the asymptotic behavior to be manifest. For the two-dimensional polygon problem in particular, it appears that the finite-lattice method has enabled us to obtain series of sufficient length that a large number of previously unanswered questions can now be answered.

In Table II we give the ratios and unbiased exponent estimates extrapolated by Neville–Aitken extrapolation. On this basis we estimate $1/y_c = 3.9708 \pm 0.0006$, and the exponent as 0.003 ± 0.006, which suggests an exact value of zero. The alternative method of analysis was based on inhomogeneous differential approximants, combined together using a previously developed statistical procedure[15,16] to give an overall estimate of the critical parameters. A summary of these approximants is shown in Table III, and they combine to yield $y_c = 0.25183 \pm 0.00003$ (or $1/y_c = 3.97093 \pm 0.0005$) with exponent -0.001 ± 0.010. We combine this analysis with the ratio analysis results to give our best estimates as $y_c = 0.251834$ and an exponent of zero, presumably corresponding to a logarithmic singularity.

Table III. Results of a Differential Approximant Analysis of the Same Series $A(y)$ Analyzed in Table II[a]

	Critical point		Critical exponent		
n	Estimate	Error	Estimate	Error	L
11	0.2509229	0.0000398	0.1586098	0.0032157	3×
12	0.2511809	0.0003948	0.1080113	0.0679823	4
13	0.2512870	0.0010713	0.0939811	0.1723455	9
14	0.2518963	0.0006981	−0.0108409	0.1145714	11
15	0.2518180	0.0002419	−0.0001454	0.0463212	11
16	0.2518924	0.0002264	−0.0137478	0.0531241	11
17	0.2517652	0.0002124	0.0171383	0.0551452	12
18	0.2518158	0.0001671	0.0038068	0.0478107	12
19	0.2518320	0.0000379	−0.0008885	0.0108081	11

[a] As in Table I, the row n indexes the coefficients corresponding to area $n+1$. Defective range factor for positive real axis: 1.200. Absolute defective range value for the complex plane: 0.005.

We have also analyzed the generating function $A(y)$ for the mean perimeter series, whose coefficient of y^n is the mean perimeter of all polygons with area n. We performed the same analysis as above, and found that $\langle p_n \rangle \sim n^g$, with $g = 1.000 \pm 0.003$. This implies that polygons are essentially linear objects, or highly ramified, as their mean perimeter is proportional to their area. Another quantity of interest is the mean area of all polygons of perimeter n, denoted $\langle a_n \rangle$, whose generating function was defined above as $\Omega(x)$. This series is also shown in Table I. By the same methods of analysis, we find $\langle a_n \rangle \sim n^p$, with $p = 1.499 \pm 0.003$, in agreement with earlier work.[3]

4. DISCUSSION

We have investigated the behavior of polygons grouped by area, rather than perimeter. For some purposes this is a more natural definition, for example, if one considers these objects as types of lattice animals or as a realization of a particular cluster counting problem. For convex polygons, row-convex polygons, and polygons we find that the exponential growth factor for the perimeter generating function is some 25–75% greater numerically than the corresponding quantity for the area generating function. It is by no means obvious that these two "critical points" should be different. The linearity of polygons, revealed by the result that $\langle p_n \rangle \sim n$, is also somewhat surprising. Another aspect that calls for further investigation is the nature of the exponent for the area generating function $A(y)$. While it is presumably logarithmic, it would be interesting to determine whether this is a simple logarithm or a more complicated structure, such as a logarithm raised to a power or a logarithm of a logarithm. Such subtleties will probably require greater analytical knowledge, but the enumerations obtained here are likely to be of value in the study of these and related questions.

NOTE ADDED IN PROOF

Row convex square lattice polygons grouped by perimeter were first discussed and partially solved by Temperley.[6] Recently Brak *et al.*[17] have obtained the generating function explicitly. Near the critical point it behaves like $A(1-\lambda x)^{1/2}$, where $\lambda = 3 + 2\sqrt{2}$. Thus λ lies between the values obtained for convex and "ordinary" square lattice polygons, as does the exponent.

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