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A new two-variable generating function for convex self-avoiding polygons

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Abstract. The width of a self-avoiding polygon on the square lattice is defined as the minimal (horizontal or vertical) distance between two of its parallel edges. If the polygons are convex, this distance is internal. The perimeter generating functions for such convex polygons, whose widths exceed a threshold, can be given explicitly. From these expressions, a two-variable (width and perimeter) generating function can be constructed. The corresponding phase diagram shows two types of critical behaviour, which meet at a tricritical point.

1. Introduction

Self-avoiding polygons (SAPs) on lattices still pose many unsolved enumeration problems which are related to spin models, see [1] for a discussion which includes the history of this type of problem. These and related enumeration problems are also important for the derivation of high-temperature series, see, e.g., [2] for the basic ideas and [3] for a more recent application to a class of complicated spin models. Some progress has been made in the last few decades. This progress consists mainly of exact results for generating functions of special classes of SAPs on the square lattice. In particular, the perimeter generating function for convex SAPs, which are such that their perimeter equals the one, P_{b} , of the smallest rectangle in which they fit, has been derived by various methods by different authors [4-7]. Several moments of the combined perimeter and area generating function have also been calculated for this case [8,9], leading finally to an expression for this function [10]. The perimeter generating function for SAPs, whose perimeter is P_b+2 , has also been found [11,12]. For SAPs with perimeters P_b+2c , variously called SAPs with concavity [13] or defect index [12] c, no further results have, as yet, been obtained for c > 1, although there are also some results for a closely connected class of lattice graphs [14]. Further classes of SAPs are the row-convex and staircase ones. For the first of these, only the width (or height) is equal to the corresponding value for the bounding rectangle. For these, the perimeter generating function is known [15] and results for the combined perimeter and area generating function have been found as well [16, 17]. The generating functions are also known [4, 17] for the staircase SAPs. These results extend the very early work of Temperley [18] and Pólya [19] for this type of SAP.

Other exact results concern the critical point $x_c^{-2} = 2 + \sqrt{2}$ and exponent $\alpha = \frac{1}{2}$ for the hexagonal lattice, although these are not rigorous [20,21]. These quantities are defined by the (assumed) singular behaviour of a perimeter generating function P(x) for $x \to x_c$:

$$P(x) = \sum_{n=0}^{\infty} p(n)x^n \sim (x_c - x)^{\alpha - 2}$$
(1.1)

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Figure 1. The definition of width of a SAP. Dashed lines indicate where the minimum is achieved.

where p(n) is the number of SAPs of a specific type with perimeter n, and x_c is the smallest value of x for which this function is singular. The exponent is thought to be universal, as is confirmed by the analysis of exact enumerations [22–25] for the square lattice. The algorithms for these have reached such a degree of sophistication that all SAPs with perimeter up to 90 have been enumerated, see the tables in [22,25].

There is an analogy between spin models and SAP problems in the following sense: the perimeter generating function can be loosely identified with the field-free free energy function of a spin model, the critical point(s) of the latter being analogous to the point x_c at which the generating function first becomes singular. Similarly, the combined perimeter and area generating function is analogous to a spin model in an external field, yielding a richer phase diagram. This analogy serves to explain the greatly increased difficulty of obtaining exact results for such two-variable functions. In this paper, a different two-variable generating function is considered, based on perimeter and *width*. This latter quantity, denoted by t, is defined as the minimum of all horizontal and vertical distances between two parallel edges of the SAP. In figure 1, three examples for t = 1, 2 and 3 are shown as examples (a)-(c), respectively. A formal definition of width is as follows.

- (i) Let V be the set of vertical edges of the SAP; a distance function d_v(e₁, e₂) for all pairs from this set can be defined by: if there is a horizontal path of length l ≥ 1 through the lattice, which contains an end vertex from both edges, then d_v(e₁, e₂) = l, else set d_v(e₁, e₂) = +∞. This latter condition applies if the edges are too far apart in the vertical direction, but also if e₁ and e₂ have a vertex in common.
- (ii) Similarly, if *H* is the set of all horizontal edges, define $d_h(f_1, f_2) = k$ if there is a vertical path of length $k \ge 1$ containing an end vertex of f_1 and of f_2 , else set $d_h(f_1, f_2) = +\infty$.
- (iii) Now the width t can be defined by

$$t = \min[\min_{e_1, e_2 \in V} d_v(e_1, e_2), \min_{f_1, f_2 \in H} d_h(f_1, f_2)].$$
(1.2)

The notion of width is not completely independent of the area, since it is clear that for a SAP with a fixed perimeter one has that:

(i) The SAP has maximal area if and only if it has maximal width.

(ii) If the SAP has minimal area it has minimal width.

Therefore, it may be expected that a combined width and perimeter generating function also shows a rich phase diagram akin to that for a spin model in an external field. On the other hand, the exact evaluation of this two-variable function may be simpler than the perimeter and area one. This provides the motivation to try such an evaluation in a simple case. In the remainder of this paper, it is shown that such an exact result can be obtained rather easily for the case of convex SAPs (CSAPs), so that an extension to concavity-1 SAPs does not look impossible.

For a perimeter and area generating function, denoted by A(x, y), the fugacities x and y can be given a physical interpretation: x is related to the surface tension (or, to be precise for

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the two-dimensional case, the line tension), whereas *y* is related to the internal pressure. In the case of a perimeter and width generating function, the second fugacity can be interpreted as measuring the strength of a local, short-range interaction between parallel edges of the SAP. This is not quite as satisfactory as in the perimeter and area case, but it should have analogous properties: if this interaction is strongly repulsive, its effect is analogous to a high internal pressure and the average SAP has large area, whereas if it is attractive, then a large perimeter is more probable as in the case of low internal pressure.

This paper is organized in the following way: in section 2, the method of describing CSAPs introduced in [12] is briefly recalled and used to obtain the perimeter generating functions for a number of subclasses. These results are used in section 3, where a method based on the repeated 'dualization' of the square lattice, which may be of independent interest, is used to obtain the perimeter generating functions $C_t(x)$ for all CSAPs with width exceeding t explicitly. These results are then used in section 4 to construct the combined perimeter and width generating function. The phase diagram corresponding to this function is derived and shown to contain two distinct phases, which join at a tricritical point. The critical exponents are also found, as well as the exact forms of all singularities. A short discussion of the results is also given.

2. Some results concerning CSAPs

It is possible to describe a CSAP of the square lattice by a set of numbers, which are related to the part of the dual lattice contained inside the CSAP [12]. The dual lattice is again square, as it is obtained from the original one by placing a vertex in each plaquette and connecting two of these if the corresponding plaquettes have an edge in common. If the CSAP fits into a bounding rectangle of dimensions $(k + 1) \times (l + 1)$, this rectangle encompasses a $k \times l$ one of plaquettes of the dual lattice; the CSAP is now completely defined by k and l and by numbers $a_1 \ge a_2 \ge \cdots \ge a_l$ and $b_1 \ge b_2 \ge \cdots \ge b_l$, which have to satisfy

$$|a_i| + |b_i| \le k$$
 for $i = 1, 2, \dots, l.$ (2.1)

The absolute value $|a_i|$ is the number of plaquettes from the dual lattice missing from the $k \times l$ rectangle on the left-hand side in the *i*th row; similarly, $|b_i|$ denotes this missing number on the right-hand side. A positive value of a_i indicates that this has been achieved by 'pushing inwards' the upper-left corner of the rectangle, whereas a negative value is used if the lowerleft corner has been 'pushed'. Similarly, b_i is positive if the upper-right corner has been used, negative if the lower-right corner has been used. All a_i and b_i can, therefore, be positive or negative, as long as their order is maintained and equation (2.1) is satisfied. An example of this numbering is shown in figure 2(a), which shows a CSAP as thin lines, and the enclosed part of the dual lattice as thick lines with vertices. Here one has k = 2, l = 3; the *a* are on the left, the b on the right. A complementary description for such a CSAP can be obtained after a rotation of the original one over $\pi/2$ in the clockwise direction; this rotated CSAP is defined by l, k and variables $a'_1 \ge a'_2 \ge \cdots \ge a'_k$, $b'_1 \ge b'_2 \ge \cdots \ge b'_k$ which satisfy an equation similar to equation (2.1) with k and l interchanged. Descriptions in primed and unprimed variables are, of course, one-to-one translatable, although this is somewhat involved and not explicitly needed in what follows. In terms of these variables, the perimeter of a CSAP is P = 2k + 2l + 4, whereas its area is

$$A = (k+1)(l+1) - \sum_{i=1}^{l} (|a_i| + |b_i|) = (k+1)(l+1) - \sum_{i=1}^{k} (|a_i'| + |b_i'|).$$
(2.2)

The width of a CSAP is simpler to define than for the general case; since all horizontal or vertical lines which go through the CSAP have exactly one piece inside it (this could actually

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Figure 2. (*a*) The notation used to describe a CSAP. (*b*) A CSAP with t = 1 and its connected double dual in (*c*). (*d*) A CSAP with t = 1 and a two-component double dual in (*e*). (*f*) A CSAP with t = 1 and its three-component double dual in (*g*). (*h*) A CSAP with t = 2, its connected double dual in (*i*) and the two-component triple dual in (*j*).

be taken as the definition of such a SAP and explains the name convex), it is just the minimum of such local, internal widths:

$$t = \min\left[\min_{1 \le i \le l} (k+1 - |a_i| - |b_i|), \min_{1 \le i \le k} (l+1 - |a_i'| - |b_i'|)\right].$$
(2.3)

As shown in [12], the number of CSAPs with a bounding rectangle given by k and l and which have their first row defined by $a = a_1, b = b_1$ is given by

$$f_k(a, b, l) = \binom{k+a+b+2l}{2l} - 2h(a) \sum_{m=1}^{\min(a,l)} \binom{a+l}{a-m} \binom{k+a+b}{l-m}$$
$$-2h(b) \sum_{m=1}^{\min(b,l)} \binom{b+l}{b-m} \binom{k+a+b}{l-m}$$
(2.4)

where the function h(x) is defined by

$$h(x) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{otherwise.} \end{cases}$$
(2.5)

The perimeter generating function follows from the numbers C(n) of CSAPs with perimeter 2n + 4,

$$C(n) = \sum_{k=0}^{n} \sum_{(a,b)} f_k(a,b,n-k)$$
(2.6)

where the brackets (a, b) signify that equation (2.1) has to be satisfied for the pair a, b. The final result is [4-7, 12]

$$C_0(x) = \sum_{n=0}^{\infty} C(n) x^n = \frac{-4x^3 + 11x^2 - 6x + 1}{(1 - 4x)^2} - \frac{4x^2}{(1 - 4x)^{\frac{3}{2}}}.$$
 (2.7)

In the following section, two more perimeter generating functions, corresponding to special subsets of CSAPs, are needed. The first of these, D(x), is the generating function for CSAPs such that the part of the dual lattice inside its bounding rectangle contains the vertex in the upper-right corner. This is equivalent to the restriction $b \leq 0$, so that this is given by the numbers

$$D_n = \sum_{k=0}^n \sum_{\substack{(a,b)\\b\leqslant 0}} f_k(a,b,n-k).$$
 (2.8)

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After some algebra, the surprisingly simple result

$$D(x) = \sum_{n=0}^{\infty} D_n x^n = (1 - 4x)^{-\frac{1}{2}}$$
(2.9)

is obtained. Also needed in the next section is the function E(x), which is the generating function of CSAPs with upper-left and lower-right corners of their dual insides occupied. This cannot be obtained directly from equations (2.4), (2.5); instead, one has to 'glue' together two SAPs of the type contributing to D(x), one upside down. The result is again rather simple:

$$E(x) = [1 - 2x - (1 - 4x)^{\frac{1}{2}}]/(2x^2).$$
(2.10)

Clearly, D(x) is also the generating function for CSAPs with any other corner of their duals occupied, whereas E(x) is also relevant to the case with the other two diagonally situated vertices occupied.

3. Results on CSAPs with width exceeding a threshold

For threshold t = 0, the perimeter generation function is just the one for all CSAPs, equation (2.7). To find the perimeter generating functions $C_t(x)$ of the CSAPs with threshold t, the case t = 1 is considered first. By definition, these CSAPs have a width larger than 1. It is easy to see that this means that there is at least one plaquette of the dual lattice left over in every row and column inside the CSAP. Examples are provided by figures 2(b), (d) and (f), which show width-2 CSAPs and by figure 2(h), which is an example of a width-3 one. This means that the duality can be repeated at least once, i.e. the procedure of placing a vertex in every plaquette and connecting these if the plaquettes have an edge in common leads to a nonempty graph again. For the examples above, this double dual graph is shown as figures 2(c), (e), (g) and (i), respectively. In the cases of figures 2(c) and (i), the resulting graphs are again connected and, as such, also directly define a CSAP; since all can be obtained in this way, these connected double dual graphs give a contribution

$$A_1(x) = x^2 C_0(x) \tag{3.1}$$

to the perimeter generating function $C_1(x)$. In the case of figure 2(d), the double dual graph of figure 2(e) has two components, each representing a CSAP with a fixed corner in its dual. Such graphs then give a contribution

$$B(x) = 2x^4 D(x)^2 (3.2)$$

to $C_1(x)$, the factor 2 stemming from the fact that these graphs can extend either from lower left to upper right, as in figure 2(d), or from upper left to lower right. In the case of figure 2(f), the double dual graph has three components. Clearly the contribution of this type of graphs to $C_1(x)$ is

$$G(x) = 2x^{6}D(x)^{2}E(x)$$
(3.3)

since the 'middle part' must have two diagonally opposite occupied corners.

It is now easy to generalize the above: for a CSAP with width larger than 1, the double dual graph is either connected or it consists of s + 2 components, $s \ge 0$, two of which have one fixed corner, the *s* others two diagonally opposed ones. The generating function for these is then, in terms of the functions D(x) and E(x),

$$C_1(x) = x^2 \bigg[C_0(x) + 2x^2 D(x)^2 \sum_{s=0}^{\infty} x^{2s} E(x)^s \bigg].$$
(3.4)

Here the *s*th term in the sum corresponds to double dual graphs with s + 2 components.

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It is not difficult to see that, for CSAPs with width larger than t > 1, the corresponding dual graphs have at least t plaquettes in every row and column. Moreover, at least t - 1 of these overlap in every pair of consecutive rows or columns. Figure 2(h) shows an example for t = 2. Therefore, the duality construction can be repeated t + 1 times, see figure 2(j) for the triple dual graph obtained from figure 2(h). This (t + 1)-dual graph can either be connected, which gives a contribution

$$A_t(x) = x^{2t} C_0(x) (3.5)$$

to the perimeter generating function $C_t(x)$, or it consists again of s + 2, $s \ge 0$ components, which are of the same types as in the case t = 1. There is a complication, due to the ways in which these can now be arranged: the overlap requirement allows all distances between occupied corners to be in the range (2, ..., t + 1), whereas if h is a distance from this range, there are h - 2 extra edges and the requirement that the resulting SAP is a CSAP allows h - 1 posibilities of arranging these corners. See also figure 2(j), where the distance between occupied corners is 3 and not 2 as in the t = 1 case. This gives rise to a factor $p_t(x)$ for every pair of consecutive components as

$$p_t(x) = \sum_{h=2}^{t+1} (h-1)x^{h-2} = \frac{tx^{t+1} - (t+1)x^t + 1}{(1-x)^2}.$$
(3.6)

For t = 0, there are no components and $p_0(x) = 0$ can be chosen for completeness. With this, the total generating function is now

$$C_t(x) = x^{2t} \bigg[C_0(x) + 2x^2 p_t(x) D(x)^2 \sum_{s=0}^{\infty} \left(x^2 p_t(x) E(x) \right)^s \bigg].$$
(3.7)

The final results of equations (3.4) and (3.7) can be rewritten as

$$C_t(x) = x^{2t} [C_0(x) + Q_t(x)] \qquad Q_t(x) = \frac{2x^2 p_t(x)}{(1 - 4x)(1 - x^2 p_t(x)E(x))}.$$
(3.8)

This is even correct for t = 0, since $p_0(x) = 0$, see equation (3.6). The leading singularity of $C_t(x)$ is always at $x_c = \frac{1}{4}$ and due to the term proportional to $C_0(x)$; this implies that the asymptotic behavour of its expansion coefficients $C_t(n)$ is

$$C_t(n) \sim n2^{2n-4t-7} [1 - 4(\pi n)^{-\frac{1}{2}} + O(n^{-1})].$$
 (3.9)

Therefore, the number of CSAPs with perimeter P = 2n + 4 and width > t is only a fraction $(\frac{1}{16})^t$ of the total number for large P.

4. The two-variable generating function

The perimeter generating function for CSAPs of width *t* exactly is, from the previous section, given by

$$R_t(x) = C_{t-1}(x) - C_t(x).$$
(4.1)

It is instructive to use the power series expansions of the $C_t(x)$ in order to obtain an insight into the number of CSAPs as functions of perimeter and width. This is done in table 1 for $P \leq 30$, for which the maximal width is 7. This table shows the asymptotic value of $\frac{1}{16}$ for the ratios $C_{t+1}(n)/C_t(n)$ as noted in equation (3.9) already clearly for t = 1 and t = 2 in the first three columns of the table. Also it can be seen that the sequences $\{C_{n+2k}(t+k)\}$ quickly increase to reach a fixed value as k increases. This is due to the fact that, for x < 1, the polynomial

	t						
Р	1	2	3	4	5	6	7
4	1						
6	2						
8	6	1					
10	26	2					
12	111	8	1				
14	492	34	2				
16	2 1 9 0	145	8	1			
18	9748	628	38	2			
20	43 244	2746	161	8	1		
22	190 940	12 000	700	38	2		
24	838742	52 342	3 0 5 2	167	8	1	
26	3 665 364	227 636	13 292	724	38	2	
28	15 938 748	986 546	57 722	3 1 6 0	167	8	1
30	68 987 824	4260076	249 852	13764	732	38	2

Table 1. The number of CSAPs $R_t(n)$ with perimeter $2n + 4 = P \leq 30$ and $t \leq 7$.

 $p_t(x)$ of equation (3.6) approaches $1/(1-x)^2$ for large t, so that a function $Q_{\infty}(x)$ can also be defined; it is given explicitly by

$$Q_{\infty}(x) = \lim_{t \to \infty} Q_t(x) = \frac{1 - 2x + 2x^2 - (1 - 4x)^{\frac{1}{2}}}{(1 - 4x)(2 - 2x + x^2)}$$
(4.2)

and its series expansion agrees with $Q_t(x)$ up to terms of order t + 1. For positive x < 1, equation (3.6) implies that $Q_t(x) < Q_{\infty}(x)$ The constant values referred to above are then the ones corresponding to the replacement of the $Q_t(x)$ by $Q_{\infty}(x)$ in equation (3.8).

The two-variable generating function C(x, y) for perimeter and width is

$$C(x, y) = \sum_{t=1}^{\infty} R_t(x) y^t = C_0(x) + (y-1) \sum_{t=0}^{\infty} C_t(x) y^t.$$
(4.3)

With equation (3.8), this becomes

$$C(x, y) = C_0(x)\frac{y(1-x^2)}{1-x^2y} + (y-1)\sum_{t=0}^{\infty} Q_t(x)(x^2y)^t.$$
(4.4)

Since $C_0(x)$ diverges at $x_c = \frac{1}{4}$, this function is majorated by $C_{\infty}(x, y)$, obtained from equation (4.4) by replacing the $Q_t(x)$ by its limit for large t for $x < x_c$, y > 1:

$$C_{\infty}(x, y) = C_0(x)\frac{y(1-x^2)}{1-x^2y} + Q_{\infty}(x)\frac{y-1}{1-x^2y}.$$
(4.5)

A rather long calculation shows that $C_{\infty}(x, y) - C(x, y)$ has no singularity at $y = x^{-2}$, where $C_{\infty}(x, y)$ is singular, but at $y = x^{-3}$. Therefore, the singularities of equation (4.4) nearest to the origin are at $x_c = \frac{1}{4}$ and at $y_c = x^{-2}$ for $x < x_c$. This phase diagram is shown as figure 3. The singularities are:

- (i) For y > 16, a simple pole (critical exponent $\mu_1 = 1$) at $x = 1/\sqrt{y}$.
- (ii) For y < 16, there is a double pole with confluent branch point singularity at x_c , due entirely to $C_0(x)$, see equation (2.7); the critical exponent is $\mu_2 = 2$.
- (iii) At the tricitical point $C = (\frac{1}{4}, 16)$, there is a triple pole (exponent $\mu_3 = 3$) with confluent branch point singularity, since the contributions from (i) and (ii) enter as a product.



Figure 3. The phase diagram of the two-variable generating function C(x, y).

It has not been possible to obtain a closed form for C(x, y); it is, however, possible to rearrange the terms so as to show the contributions from the different types of CSAP and to give some information on the complete singularity structure. To this end, the expanded versions for $C_t(x)$ of equations (3.4) and (3.7) are inserted into equation (4.3); the result is

$$C(x, y) = C_1(x, y) + \frac{2x^2(y-1)}{1-4x} \sum_{s=0}^{\infty} [x^2 E(x)]^s F_{s+1}(x, x^2 y)$$

$$C_1(x, y) = C_0(x) \frac{y^2(1-x^2)}{1-x^2 y}$$

$$F_s(x, z) = \sum_{t=1}^{\infty} p_t(x)^s z^t.$$
(4.6)

Here the term $C_1(x, y)$ derives from connected maximally dualized graphs, whereas the sth term in the sum derives from maximally dualized graphs with s + 2 components. By writing the explicit form of $p_t(x)$, equation (3.6), for one of the factors in the last equation above, a recursion relation for the functions $F_s(x, z)$ can be derived:

$$F_s(x,z) = [F_{s-1}(x,z) - F_{s-1}(x,xz)]/(1-x)^2 - xzF'_{s-1}(x,xz)/(1-x).$$
(4.7)

Here $F'_s(x, z)$ is the partial derivative of $F_s(x, z)$ with respect to z; the startpoint of the recursion is, from the last of equations (4.6), $F_0(x, z) = z/(1 - z)$. From this recursion, it follows that these functions have the form of polynomials $G_{x}(x, z)$ in x and z, divided by a product of factors:

$$F_s(x,z) = G_s(x,z) \left[\prod_{i=1}^{s+1} (1-x^{i-1}z)^i \right]^{-1}.$$
(4.8)

Therefore, if the singularities of C(x, y) are due to those of the F_s -functions (this is, of course, difficult to ascertain, since there is still an infinite sum in equation (4.6)), they fall into three classes, which are analogous to the ones found nearest the origin:

- (i) For y > 4^{s+1}, s = 1, 2, ..., there is an *s*-fold pole at x^{s+1} = 1/y.
 (ii) For y < 4^{s+1}, s = 1, 2, ..., there still is only a double pole with confluent branch point singularity at $x = \frac{1}{4}$.

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(iii) For $y = 4^{s+1}$, $x = \frac{1}{4}$, there is an (s+2)-fold pole with confluent branch point singularity.

It is not very easy to compare the present results with the exact perimeter and area one [10], since in this paper no phase diagram has been extracted from the (very complicated) final result. The structure of this result is, however, similar to the one of equation (4.8); this is also the case for the other exactly solved cases [16, 17]. In particular, the numerical phase diagram in [16] for the row-convex polygons looks qualitatively similar to figure 3. Therefore, it seems that the two-variable generating function presented in this paper captures the essential features of the perimeter and area one without it being as complicated to evaluate, at least for CSAPs. An extension to SAPs with concavity 1 (see section 1) may be possible and will be attempted.

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