Scaling function for self-avoiding polygons

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December 13, 2002

Abstract

Exactly solvable models of planar polygons, weighted by perimeter and area, have deepened our understanding of the critical behaviour of polygon models in recent years. Based on these results, we derive a conjecture for the exact form of the critical scaling function for planar self-avoiding polygons. The validity of this conjecture was recently tested numerically using exact enumeration data for small values of the perimeter on the square and triangular lattices. We have substantially extended these enumerations and also enumerated polygons on the hexagonal lattice. We also performed Monte-Carlo simulations of the model on the square lattice. Our analysis supports the conjecture that the scaling function is given by the logarithm of an Airy function.

1 Introduction

The model of self-avoiding polygons (SAPs) is an important unsolved combinatorial problem in statistical mechanics [23, 13]. In this article, we consider the model of SAPs in two dimensions. SAPs counted by perimeter are the canonical model of ring polymers, while when also counted by area, they serve as a model of vesicles [20]. The model also has connections with many other models of statistical mechanics where boundaries of certain cluster types play a role, notably in percolation and in spin models such as the Ising model and the Potts model, see also [7]. Despite its importance, there are only a few known rigorous results about SAPs, almost all information arising from numerical investigations [11, 23, 11, 13, 8, 4]. Promising new developments however arise from the theory of stochastic processes [18], see also [6] (this volume). Recently, we verified numerically a conjecture of one of us about the scaling function for SAPs, which describes the singular part of the SAP perimeter and area generating function about its tricritical point [35, 36]. The prediction of the scaling function also gives the distribution of area moments. The conjecture was already stated in 1995 [31], as a result of a systematic investigation of simple exactly solvable subclasses of SAPs. There it was noticed that the critical exponents of *rooted* SAPs coincide with the exponents of staircase polygons, where the scaling function had been computed [28]. This led to the question whether both scaling functions are of the same type.

Over the years, it turned out that the mathematical structure underlying exact solvability is given by q-algebraic functional equations. They arise from the requirement that the polygon model is built up recursively, see e.g. [1]. This general type of functional equation appears first, within the framework of algebraic languages, in [9], together with the discussion of the area distribution for simple polygon models showing a square-root singularity. However, the article [9] does not contain a derivation of its central result. Recently, we investigated the scaling behaviour of general q-algebraic functional equations [35, 36] and noticed that it generically depends only on the singularity of the perimeter generating function. This remarkable kind of universality further supported the above conjecture and led us to test it numerically.

Very recently, investigations on the self-avoiding walk problem using the theory of stochastic processes led to a number of predictions of the behaviour of SAPs in the scaling limit. One of them is that the scaling limit of the half plane infinite SAP is the outer boundary of the union of two Brownian excursions from 0 to ∞ in the upper half plane [18]. Since the area under a Brownian excursion is Airy distributed [21], this would suggest that the area moments of SAPs obey an Airy type distribution. This is consistent with our conjecture that the SAP scaling function is the logarithm of an Airy function and also illuminates the connection with the model of staircase polygons, whose scaling limit is described by Brownian excursions.

In the remainder of this article we first introduce polygon models, in particular self-avoiding polygons, and discuss their critical behaviour. We then consider q-algebraic functional equations and show how to extract scaling behaviour in the vicinity of a square-root singularity from the functional equation. The following section analyses the exactly solvable example of bar-graph polygons, using the techniques described in the previous section. The next section on self-avoiding polygons contains a summary of the analysis of recently obtained exact enumeration data for polygons on the square lattice to perimeter 100, the hexagonal lattice to perimeter 140 and the triangular lattice to perimeter 58. The analysis confirms the conjectured form of the scaling function in that predicted exact amplitude combinations are confirmed to within a numerical accuracy of 5–6 significant digits. This section also explains the Monte-Carlo simulation method, which we performed on the square lattice for polygons up to perimeter 2048, and confirms the conjectured form of the scaling function within a numerical accuracy of 3 significant digits. A concluding section discusses possible applications of our results and methods.

2 Polygon models and their scaling behaviour

For concreteness, we discuss models of polygons defined on the square lattice $\mathbb{Z}^2$. These models can be defined similarly for other lattices as well as in the continuous case. A *self-avoiding polygon (SAP)* is a closed, non-intersecting loop on the edges of the square lattice. Important subclasses are *staircase polygons* and *bar-graph polygons* [29], whose obvious definition may be extracted from Figure 1. Whereas the latter two models have been solved exactly, as also discussed below, for

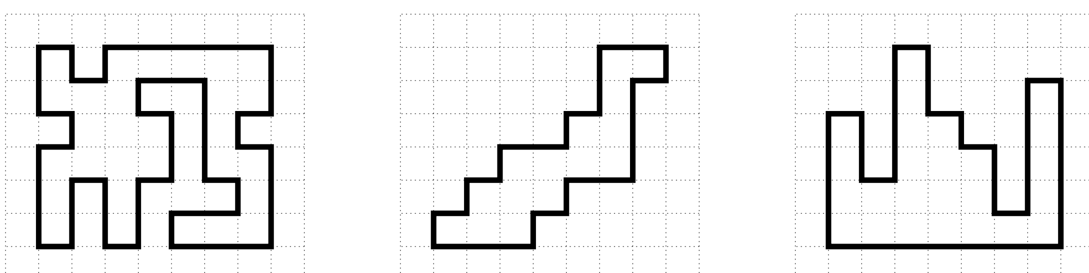

Figure 1: Prominent polygon models. ¿From left to right: self-avoiding polygons, staircase polygons, bar-graph polygons.

SAPs there are very few rigorous results, complemented by a number of numerical investigations. Let $p_{m,n}$ denote the number of different polygons of perimeter m and area n, respectively, where we regard translated polygons as equal. The object of interest is the *perimeter and area generating function*

$$G(x,q) = \sum_{m,n} p_{m,n} x^m q^n, \tag{2.1}$$

where we introduced a perimeter activity x and an area activity q. Sometimes, horizontal and vertical perimeter are distinguished, leading to an anisotropic perimeter and area generating function $G(x,y,q)$. The function $G(x,1)$ is called *perimeter generating function.* Of particular interest is the singular behaviour of $G(x,q)$ as a function of x and q, which translates to the behaviour of the coefficients $p_{m,n}$ in the limit of large perimeter and area.

The above models display a so-called *collapse transition* between a phase of extended and a phase of deflated polygons [11]: in the extended phase $q=1$, the mean area of polygons $\langle a\rangle_m$ of perimeter m grows asymptotically like $m^{3/2}$, whereas it grows like m in the deflated phase $q<1$. It can be shown that in the limit $q\to 0$ the generating function is dominated by polygons of minimal area. Since for SAPs these polygons may be viewed as branched polymers, the phase $q<1$ is also referred to as the *branched polymer phase.* This change of asymptotic behaviour is reflected in the singular behaviour of the perimeter and area generating function. Typically, the line $q=1$ is a line of finite essential singularities for $x<x_c$. The line $x_c(q)$, where $G(x,q)$ is singular for $q<1$, is typically a line of algebraic (staircase, bar-graph) or logarithmic (SAPs) singularity. For branched polymers in the continuum limit, the logarithmic singularity has been recently proved in [3] (see also this volume).

Of special interest is the point $(x_c,1)$ where these two lines of singularities meet. The behaviour of the singular part of the perimeter and area generating function about $(x_c,1)$ is expected to take the special form

$$G(x,q)\sim G^{(reg)}(x,q)+(1-q)^{\theta}F((x_c-x)(1-q)^{-\phi}),\qquad (x,q)\to(x_c^-,1^-),\tag{2.2}$$

where $F(s)$ is a *scaling function* of combined argument $s=(x_c-x)(1-q)^{-\phi}$, commonly assumed to be regular at the origin, and θ and ϕ are *critical exponents.* The singular behaviour about $q=1$ at the critical point x_c is then given by $G^{(sing)}(x_c,1)\sim(1-q)^{\theta}F(0)$. This scaling assumption implies an asymptotic expansion of the scaling function of the form

$$F(s)=\sum_{k=0}^{\infty}\frac{f_k}{s^{(k-\theta)/\phi}}.\tag{2.3}$$

The leading asymptotic behaviour characterises the singularity of the perimeter generating function via $G(x,1)\sim f_0(x_c-x)^{-\gamma}$, where $\theta+\phi\gamma=0$. The first singularity of $F(s)$ on the negative axis determines the singularity along the curve $x_c(q)$. The locus on the axis (say at $s=s_c$) determines the line $x_c(q)\sim x_c-s_c(1-q)^{\phi}$ near $q=1$, which meets the line $q=1$ vertically for $\phi<1$.

The area moments $g_k(x)$ are defined as coefficients of the (formal) expansion of the generating function about $q=1$

$$G(x,q)=\sum_k g_k(x)(1-q)^k,\qquad g_k(x)=\frac{(-1)^k}{k!}\sum_{m,n}n(n-1)\cdots(n-k+1)p_{m,n}x^m.\tag{2.4}$$

Note that $g_0(x)=G(x,1)$ is the perimeter generating function. The higher moments $g_k(x)$ can be computed recursively using $g_l(x)$, where $l<k$ using the functional equation [36]. There is an important relation between the scaling function and the area moments: The coefficients f_k in the asymptotic expansion of the scaling function are the leading singular amplitudes of the area moments $g_k(x)$. This follows from the scaling assumption which implies that the leading singular behaviour of the area moments is of the form

$$g_k^{(sing)}(x)\sim\frac{f_k}{(x_c-x)^{\gamma_k}}\qquad (x\to x_c^-),\tag{2.5}$$

where $\gamma_k=(k-\theta)/\phi$. Thus, information about the scaling function can be obtained from the leading singular behaviour of the area moments which are, in turn, obtainable by a numerical analysis, extrapolating finite-size data.

3 q-Algebraic functional equations

Due to the difficulty of the SAP problem, simple subclasses of SAPs have been analysed in the past; for example rectangles, Ferrers diagrams, stacks, staircase polygons, bar-graph polygons, convex polygons and column-convex polygons, among others [1, 2, 29, 31]. All these models share the special property that they are directed, i.e. they can be thought of as being built up by adding consecutive layers of squares. This results in a special recursion for the coefficients $p_{m,n}$ or a specific functional equation for the generating function $G(x,q)$. Over the years it has become clear that the underlying structure is a *q-algebraic functional equation* of the form

$$P(G(x,q), G(qx,q), \ldots, G(q^N x,q), x, q) = 0, \tag{3.1}$$

where $P(y_0, y_1, \ldots, y_N, x, q)$ is a polynomial in $y_0, y_1, \ldots, y_N, x$ and q. All exactly solved polygon models satisfy such a functional equation (with x conjugate to the (horizontal) perimeter and q conjugate to the area). For the example of bar-graph polygons, see the next section. No such recursion is known for SAPs, however. The limit $q \to 1$ in (3.1) generally leads to an *algebraic* differential equation, i.e. an algebraic equation in x, $G(x,1)$ and its derivatives. The exactly solved polygon models, however, result in a purely algebraic equation, i.e. in the non-trivial polynomial identity

$$P(G(x,1), G(x,1), \ldots, G(x,1), x, 1) = 0. \tag{3.2}$$

Not much is known about the singular behaviour of general q-algebraic functional equations. The q-linear case, however, has been treated in some detail, see [34] and references therein. The polygon models of rectangles, Ferrers diagrams, and stacks are q-linear [30], whereas the other exactly solved models cited above satisfy q-quadratic functional equations. Using (3.2), we see that the perimeter generating function $G(x,1)$ displays an algebraic singularity at some point x_c. The most direct way to extract the scaling function about $x = x_c$ and $q = 1$, whose existence we assume, from the defining q-functional equation, is to insert the Ansatz (2.2) into the functional equation, introduce the scaling variable $s = (x_c - x)(1-q)^{-\phi}$ and expand the functional equation to leading order in $\epsilon = 1 - q$. This will, to lowest order in ϵ, result in a differential equation for the scaling function $F(s)$. Above method is also called method of *dominant balance* [29]. Note first that the expansion of the generating function with q-shifted argument is given to leading order by

$$G(q^k x, q) = G^{(reg)}(x,q) + \epsilon^\theta F(s) + k x_c \epsilon^{\theta + (1-\phi)} F'(s) + \mathcal{O}(\epsilon^{\theta + 2(1-\phi)}). \tag{3.3}$$

We will analyse the case of a square-root singularity of the perimeter generating function in detail. (The case of a simple pole is discussed in [36]). It imposes the restrictions

$$P = 0, \qquad \left(\sum_k \partial_k P\right) = 0, \qquad \left(\sum_{k,l} \partial_{k,l} P\right) \neq 0, \qquad (\partial_x P) \neq 0 \tag{3.4}$$

on the functional equation, evaluated at $(x,q) = (x_c, 1)$. We introduced the abbreviations $\partial_k = \partial_{y_k}$ and $\partial_{k,l} = \partial_{y_k}\partial_{y_l}$ for $0 \leq k, l \leq N$. The assumption of a square-root singularity also implies $\phi = 2\theta$ for the critical exponents, as follows from the relation $\theta + \phi\gamma = 0$. The functional equation then has an expansion of the form

$$0 = \epsilon^{2\theta} \frac{1}{2} \left(\sum_{k,l} \partial_{k,l} P\right) F^2(s) + \epsilon^{\theta + (1-\phi)} x_c \left(\sum_k k \partial_k P\right) F'(s) - \epsilon^\phi (\partial_x P)\, s + \cdots \tag{3.5}$$

to lowest orders in ϵ. In order to obtain a non-trivial equation for the scaling functions, we demand equality of the coefficients. This results in exponents $\theta = 1/3$ and $\phi = 2/3$, and we get the Riccati equation

$$F(s)^2 - 4 f_1 F'(s) - f_0^2 s = 0, \tag{3.6}$$

where the coefficients f_0 and f_1 are given by

$$f_0^2 = \frac{(\partial_x P)}{\frac{1}{2}\left(\sum_{k,l} \partial_{k,l} P\right)}, \qquad -4 f_1 = x_c \frac{\left(\sum_k k \partial_k P\right)}{\frac{1}{2}\left(\sum_{k,l} \partial_{k,l} P\right)}. \tag{3.7}$$

The equation, together with the prescribed asymptotic behaviour, has the unique solution

$$F(s) = -4f_1 \frac{d}{ds} \ln \mathrm{Ai}\left(\left(\frac{f_0}{4f_1} \right)^{2/3} s \right), \tag{3.8}$$

where $\mathrm{Ai}(x) = \frac{1}{\pi}\int_0^\infty \cos(t^3/3 + tx)\, dt$ is the Airy function. The scaling function is regular at the origin, and its first singularity on the negative real axis is a simple pole, located at $\left(\frac{f_0}{4f_1}\right)^{2/3} s_c = -2.338107\ldots$.

It is important to notice that the functional form of the result is *independent* of the detailed form of the functional equation, as long as the coefficients f_0 and f_1 are nonzero and finite! Thus, the scaling behaviour is determined by the type of singularity of the perimeter generating function. This remarkable kind of universality allows us to conjecture the functional form of the scaling function for self-avoiding polygons: Together with the (numerical) observation that the perimeter generating function of the model of *rooted* SAPs $G^{(r)}(x, q) = x\frac{d}{dx}G(x, q)$ also has a square-root singularity, one might ask if it has the scaling function (3.8).

4 Bar-graph polygons

The model of bar-graph polygons has been defined and solved exactly in [29]. We review the derivation and extract the scaling behaviour as outlined above. Let $G(x, y, q)$ denote the anisotropic perimeter and area generating function for bar-graph polygons. The variable q is conjugate to the area, while the variables x and y are conjugate to the horizontal and vertical perimeters respectively. By partitioning the set of bar-graph polygons into subsets of inflated and concatenated ones, it is straightforward to show that $G(x, y, q)$ satisfies a q-quadratic functional equation in the horizontal perimeter variable x and the area variable q

$$G(x, y, q) = yG(qx, y, q)\, qx\, G(x, y, q) + y\, G(qx, y, q)\, qx + y\, G(qx, y, q) + qx\, G(x, y, q) + y\, qx. \tag{4.1}$$

This is depicted in Figure 2. The q-quadratic functional equation can – similarly to the treatment

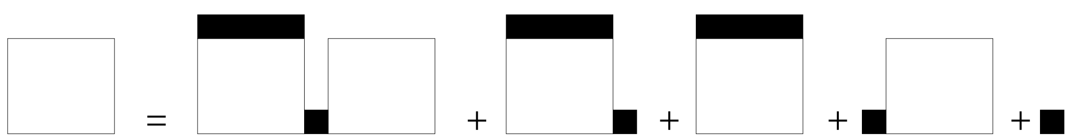

Figure 2: Diagrammatic representation of the bar-graph polygons functional equation [29].

of a Riccati differential equation – be linearised by means of the transformation

$$G(x, y, q) = \frac{y}{qx}\left(\frac{H(qx, y, q)}{H(x, y, q)} - (1 + qx) \right), \tag{4.2}$$

and the resulting q-linear functional equation of order two for $H(x, y, q)$ can be solved by iteration. This leads to

$$H(x, y, q) = \sum_{n=0}^{\infty} \frac{(-qx(1-y))^n q^{\binom{n}{2}}}{(q; q)_n (y; q)_n}, \tag{4.3}$$

where $(t; q)_n = \prod_{k=0}^{n-1}(1 - tq^k)$ denotes the q-product. The appearance of a q-series is a generic feature of solutions of q-algebraic functional equations, making it difficult to extract the asymptotic behaviour for $q \to 1$ directly from an exact solution. For staircase polygons, the first exactly solved model with a q-quadratic functional equation [2, 29], this has been done by use of saddle point techniques [28], and this method can also be applied to the above solution. A more direct approach consists in deriving the (anisotropic) scaling function directly from the defining functional equation by use of the above methods. To this end, note that the defining polynomial is of the form $P(z_0, z_1, x, q) = qxyz_1z_0 + (1+qx)yz_1 + (qx-1)z_0 + qxy$. The perimeter generating function may be found by setting $q = 1$ and solving the functional equation for $G(x, 1)$. It has a square-root singularity at $x_c = \frac{1-y}{1+3y}$. An analysis along the above lines yields

$$f_0^2 = \frac{(1+3y)^2}{y(1-y)}, \qquad -4f_1 = \frac{3+y}{1+3y}, \tag{4.4}$$

and the scaling function is the logarithmic derivative of an Airy function, given by (3.8). The critical exponents are $\theta = 1/3$ and $\phi = 2/3$.

5 Self-avoiding polygons

The model of *rooted* SAPs, $G^{(r)}(x, q) = x\frac{d}{dx}G(x, q)$, has been analysed numerically some time ago, where it was found to exhibit the same exponents $\theta = 1/3$ and $\phi = 2/3$ as bar-graph (staircase) polygons which, in particular, implies a square-root singularity of the perimeter generating function (see also [14]). With the improved series data now at hand and the refined techniques of analysis, we were able to confirm our conjecture about the scaling function to high precision using data obtained from exact enumeration for small values of perimeter, on the square lattice and on the triangular lattice [35]. In addition, it allowed us to analyse the first two corrections to scaling [36]. Here, we present results obtained from an analysis of extended enumeration data for square, hexagonal and triangular lattices and in addition we present data for the square lattice obtained from Monte-Carlo simulations. The underlying assumption is that the scaling behaviour of rooted SAPs may be arbitrarily well approximated by the scaling behaviour of solutions to a q-algebraic functional equation with a square-root singularity. The scaling function (3.8) implies certain relations between the amplitudes f_k of the leading singularity (2.5) of the area moment functions $g_k(x)$. Using the Riccati equation (3.6) for the scaling function, it can be shown that $f_n = c_n f_1^n f_0^{1-n}$, where the numbers c_n are given by the quadratic recursion

$$c_n + (3n-4)c_{n-1} + \frac{1}{2}\sum_{r=1}^{n-1} c_{n-r}c_r = 0, \qquad c_0 = 1. \tag{5.1}$$

The first few values are $c_1 = 1$, $c_2 = -5/2$, $c_3 = 15$, $c_4 = -1105/8$, $c_5 = 1695$, $c_6 = -414125/16$, $c_7 = 472200$, $c_8 = -1282031525/128$, $c_9 = 242183775$, $c_{10} = -1683480621875/256$. The coefficients f_k may be estimated from series enumeration data: Assuming an asymptotic growth of coefficients of the area moment functions $g_k(x)$ of rooted SAPs of the form

$$[x^m]g_k(x) \sim (-1)^k E_k x_c^{-m} m^{\gamma_k - 1} \qquad (m \to \infty) \tag{5.2}$$

implies a singular behaviour of $g_k(x)$ of the form (2.5) with $f_k = (-1)^k \frac{E_k}{\sigma} x_c^{\gamma_k}\Gamma(\gamma_k)$ and $\gamma_k = (3k-1)/2$. The constant σ is defined such that $p_{m,n}$ is nonzero only if m is divisible by σ. Thus $\sigma = 2$ for the square and hexagonal lattices and $\sigma = 1$ for the triangular lattice. Note that the amplitudes E_k, defined by (5.2), take the same values for rooted SAPs and for (ordinary) SAPs. Extrapolation techniques allow us to estimate x_c, γ_k and E_k to high precision. This route was followed in [35, 36] where we used series data from exact enumeration up to perimeter 86 on the square lattice and up to perimeter 29 on the triangular lattice, where the same behaviour (5.2) is expected due to universality.

Since then the enumeration of area-moments for square lattice SAPs has been extended to perimeter 100 (110) [15], and series have been derived for the hexagonal lattice to perimeter 140 (156) and the triangular lattice to perimeter 58 (60) [16], where the numbers in parenthesis refer to slightly longer series calculated for the perimeter generating function. Details of analysis can be found in [17, 14] and a brief summary will suffice here. Estimates for the critical points and exponents are obtained using the numerical technique of differential approximants [12]. For the square and hexagonal lattices, where $\sigma = 2$ and only coefficients with m even are non-zero, we

Amplitude	Exact value	Square	Hexagonal	Triangular
E_0	unknown	0.56230130(2)	1.27192995(10)	0.2639393(2)
E_1	0.7957747×10^{-1}	$0.795773(2) \times 10^{-1}$	$0.795779(5) \times 10^{-1}$	$0.795765(10) \times 10^{-1}$
E_2E_0	0.3359535×10^{-2}	$0.335952(2) \times 10^{-2}$	$0.335957(6) \times 10^{-2}$	$0.335947(5) \times 10^{-2}$
$E_3E_0^2$	0.1002537×10^{-3}	$0.100253(1) \times 10^{-3}$	$0.100255(3) \times 10^{-3}$	$0.100251(4) \times 10^{-3}$
$E_4E_0^3$	0.2375534×10^{-5}	$0.237552(2) \times 10^{-5}$	$0.237557(7) \times 10^{-5}$	$0.237547(6) \times 10^{-5}$
$E_5E_0^4$	0.4757383×10^{-7}	$0.475736(3) \times 10^{-7}$	$0.475749(10) \times 10^{-7}$	$0.475724(15) \times 10^{-7}$
$E_6E_0^5$	0.8366302×10^{-9}	$0.836624(5) \times 10^{-9}$	$0.836652(10) \times 10^{-9}$	$0.83660(2) \times 10^{-9}$
$E_7E_0^6$	$0.1325148 \times 10^{-10}$	$0.132514(2) \times 10^{-10}$	$0.132519(5) \times 10^{-10}$	$0.132511(5) \times 10^{-10}$
$E_8E_0^7$	$0.1924196 \times 10^{-12}$	$0.192418(2) \times 10^{-12}$	$0.192426(8) \times 10^{-12}$	$0.192419(8) \times 10^{-12}$
$E_9E_0^8$	$0.2594656 \times 10^{-14}$	$0.259464(2) \times 10^{-14}$	$0.259472(12) \times 10^{-14}$	$0.25948(4) \times 10^{-14}$
$E_{10}E_0^9$	$0.3280633 \times 10^{-16}$	$0.328062(4) \times 10^{-16}$	$0.328051(15) \times 10^{-16}$	$0.32812(5) \times 10^{-16}$

Table 1: Predicted exact values for universal amplitude combinations and estimates from enumeration data for square, hexagonal and triangular lattice polygons.

actually analyse the functions $h_k(y) = \sum_{m\geq 0,n} n^k p_{2m+j,n} y^m$, where $j = 4$ and 6 is the perimeter of the smallest SAP on the square and hexagonal lattices, respectively. A singularity at $x = x_c$ in $g_k(x)$ thus becomes a singularity at $y = x_c^2$ in $h_k(y)$. The generating functions for the square and triangular lattices show no convincing signs of singularities other than the one at x_c. In these cases we fit the coefficients to the assumed form

$$p_m a_m^{(k)} = \sum_n n^k p_{m,n} \sim x_c^{-m} m^{\gamma_k - 1} k! [E_k + \sum_{i\geq 0} a_i / m^{1+i/2}] \qquad (m \to \infty). \tag{5.3}$$

In the hexagonal case $h_k(y)$ has an additional singularity on the negative axis at $y = -x_-^2 = -0.412305(5)$ with exponents which appear to equal the exponents at $y = x_c^2 = 0.2928932\ldots$, as first noted in [10]. Since $x_- > x_c$ the singularity at $y = -x_-^2$ is exponentially suppressed as $m \to \infty$, however for small values of m it still has a significant influence on the coefficients in the generating functions and we have to add an extra sequence to the fit similar to (5.3):

$$(-1)^{m/2} |x_-|^{-m} m^{\gamma_k - 1} k! [E_- + \sum_{i\geq 0} b_i / m^{1+i/2}].$$

We obtain several data sets by varying the number of terms used in the fit. Only the even coefficients are used in these fits for square and hexagonal SAPs. To obtain the final estimates we do a simple linear regression on the data for the amplitudes as a function of $1/m$ extrapolating to $1/m \to 0$. We estimate the error in the amplitude from the spread among the different data sets. In this way, we obtain the results for the amplitude combinations listed in Table 1, which have been shown to be independent of the underlying lattice [8, 35]. The scaling function prediction for these numbers is

$$E_{2k} E_0^{2k-1} = -\frac{c_{2k}}{4\pi^{3k}} \frac{(3k-2)!}{(6k-3)!}, \qquad E_{2k+1} E_0^{2k} = \frac{c_{2k+1}}{(3k)! \pi^{3k+1} 2^{6k+2}} \tag{5.4}$$

for $k \in \mathbb{N}$, where we used the known result that $E_1 = \frac{1}{4\pi}$ [4], and the numbers c_k are defined in (5.1). It is clear that the estimates for the first 10 area weighted moments are in perfect agreement with the predicted exact values.

We also extended our previous approach by analysing SAPs up to perimeter 2048 by a Monte-Carlo simulation. An effective method of Monte-Carlo SAP generation of a given perimeter m has been described in [22]. Each MC step consists of an inversion or a certain reflection of a randomly chosen part of the SAP. Polygons which are no longer self-avoiding are rejected. The check for self-avoidance (by marking the corresponding lattice points) as well as the area determination ("on the fly") can be done in time proportional to the polygon length. For a given perimeter m, we took a sample of 10^6 polygons, with at least $10 \times m$ MC update moves between consecutive measurements. This leads to an estimated statistical error of 1 part in 1000. For perimeter 2048, this took two days of CPU time on a 1.5 GHz PC. We used the random number generator `ran2` described in [33]. ¿From the Monte-Carlo measurements of polygons of a given perimeter m, we extracted ratios D_k/D_1^k of the mean area moment amplitudes D_k defined by

$$\langle a^k \rangle_m = \frac{\sum_n n^k \tilde{p}_{m,n}}{\sum_n \tilde{p}_{m,n}} \sim D_k k! m^{2k\nu} \qquad (m \to \infty), \tag{5.5}$$

where $\tilde{p}_{m,n}$ is the number of sampled polygons of area n, and $\nu = 3/4$ follows from (5.2). Note that by using MC sampling we cannot measure the coefficients E_k of (5.2) directly but only the ratios $D_k = E_k/E_0$. We tested the accuracy of the random number generator by comparing values for the area moments obtained by simulation with their exact values, which are available up to perimeter 100 from exact enumeration. Assuming the above scaling function results, for $k \in \mathbb{N}$, in the values for the amplitude ratios

$$D_{2k}/D_1^{2k} = -c_{2k} \frac{(3k-2)! 2^{4k-2}}{(6k-3)! \pi^k}, \qquad D_{2k+1}/D_1^{2k+1} = c_{2k+1} \frac{1}{(3k)! 2^{2k} \pi^k}, \tag{5.6}$$

where the numbers c_k are defined in (5.1). We computed the values $\langle a^k \rangle_m / (k! \langle a \rangle_m^k)$ for $m = 64, 96, 128, 192, 256, 512, 1024, 2048$, and a typical data plot is shown in Figure 3.

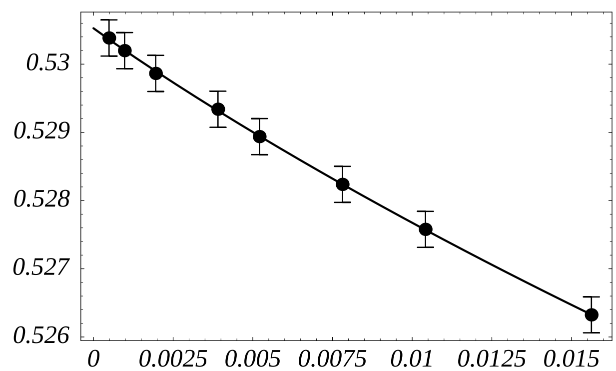

Figure 3: MC estimates of $\langle a^2 \rangle_m / (2\langle a \rangle_m^2)$ plotted against $1/m$. The estimated statistical relative error is one part in 1000.

We then extrapolated the numbers D_k/D_1^k by a least squares fit to $\langle a^k \rangle_m / (k! \langle a \rangle_m^k) \sim D_k/D_1^k + a_1 m^{-1} + a_2 m^{-3/2}$ as $m \to \infty$, in analogy with the series extrapolation for exact enumeration data. The corresponding results for the first ten amplitude combinations are given in Table 2, together with their theoretical values. The relative error is less than 1 part in 1000.

The value of D_1 is estimated to be $D_1 \approx 0.141776$. We can compare this to our previous analysis by noting that $D_1 = E_1/E_0 \approx 0.14152105(1)$, where $E_1 = \frac{1}{4\pi}$ has been derived by conformal field theory arguments [8], and $E_0 = 0.56230130(2)$ together with $x_c = 0.379052277757(5)$ has been determined in [17, 14, 15]. Noting that $f_0 = -2\frac{E_0}{\sigma}\sqrt{\frac{\pi}{x_c}}$ and $f_1 = -x_c \frac{E_1}{\sigma} = -\frac{x_c}{4\pi\sigma}$ we arrive at the conjectured form of the scaling function for rooted SAPs

$$F^{(r)}(s) = \frac{x_c}{\pi\sigma} \frac{d}{ds} \log \mathrm{Ai}\left(\frac{\pi}{x_c} (2E_0)^{\frac{2}{3}} s \right) \tag{5.7}$$

with exponents $\theta = 1/3$ and $\phi = 2/3$. (Formula (22) in [35] is correct up to a minus sign.) The conjectured form of the scaling function is then obtained by integration and is

$$F(s) = -\frac{1}{\pi\sigma} \log \mathrm{Ai}\left(\frac{\pi}{x_c} (2E_0)^{\frac{2}{3}} s \right) \tag{5.8}$$

Amplitude	Exact value	MC data
D_2/D_1^2	0.530516×10^{-0}	0.530526×10^{-0}
D_3/D_1^3	0.198944×10^{-0}	0.198954×10^{-0}
D_4/D_1^4	0.592380×10^{-1}	0.592445×10^{-1}
D_5/D_1^5	0.149079×10^{-1}	0.149105×10^{-1}
D_6/D_1^6	0.329452×10^{-2}	0.329534×10^{-2}
D_7/D_1^7	0.655743×10^{-3}	0.655959×10^{-3}
D_8/D_1^8	0.119654×10^{-3}	0.119705×10^{-3}
D_9/D_1^9	0.202754×10^{-4}	0.202863×10^{-4}
D_{10}/D_1^{10}	0.322149×10^{-5}	0.322376×10^{-5}

Table 2: Comparison of prediction for amplitude ratios against MC data. The estimated statistical relative error is one part in 1000.

with exponents $\theta = 1$ and $\phi = 2/3$. The parameters for the hexagonal lattice are $\sigma = 2$ and $x_c = 1/\sqrt{(2+\sqrt{2})}$ (known exactly from the work of Nienhuis [25]) and for the triangular lattice $\sigma = 1$ and $x_c = 0.2409175745(3)$.

6 Conclusion

We discussed the scaling behaviour of q-algebraic functional equations which underlie the critical behaviour of exactly solvable planar polygon models, counted by perimeter and area. This led to a prediction of the scaling function of the unsolved model of self-avoiding polygons on the square lattice, which we verified to numerical precision. The prediction also implies certain amplitude combinations for all area moments. It was previously argued [8] that these combinations should be universal, i.e., independent of the underlying lattice. Our investigations on the triangular and on the hexagonal lattices support the universality hypothesis, see also [35]. It is possible to extend the above analysis to include the first few corrections to scaling [36].

The question arises whether the SAP area statistics can be found in other models as well. One candidate is the hull of planar Brownian motion, which was observed in 1984 to have the same fractal dimension as SAPs [24]. Interestingly, this observation has been proved recently using methods of stochastic processes [19]. It might thus be possible to derive the area distribution rigorously for this model, as well as a corresponding prediction for the SAP area distribution.

Since q-algebraic functional equations are the underlying mathematical structure of (exactly solvable) planar polygon models counted by perimeter and area, they may serve to classify possible scaling behaviour of these polygon models. q-algebraic functional equations exhibit various types of scaling behaviour, depending on the specific type of singularity of the perimeter and area generating function [36]. Since the techniques applied so far only make use of formal power series expansions, one might ask for a proof of existence of a uniform asymptotic expansion. Details of a proof may rely on techniques used in the related problem of the behaviour of differential equations containing a parameter [26] about singular points. Recently, the scaling function prediction has been rederived using field-theoretic methods and generalised to higher order critical points [5]. It would be interesting to see whether the proposed scaling functions of [5] arise in this framework as well. It may be possible that q-algebraic functional equations also provide insight into models of polygons with interaction, q then being the activity of interaction. There is at least one such exactly solvable model: self-interacting partially directed walks [27].

Another possible application might be to models of cluster hulls, which appear in percolation or in spin models as boundaries of spin clusters in the Ising model or in the Potts model, as described in [7].

Acknowledgements

CR would like to acknowledge financial support by the German Research Council (DFG). IJ and AJG would like to acknowledge the Australian Research Council (ARC) and IJ would also like to thank the Australian Partnership for Advanced Computing (APAC) and the Victorian Partnership for Advanced Computing (VPAC) for generous allocations of computational resources.

References

[1] Bousquet-Mélou M 1996 A method for the enumeration of various classes of column-convex polygons *Discr. Math.* **154** 1-25

[2] Brak R and Guttmann A J 1990 Exact solution of the staircase and row-convex polygon perimeter and area generating function *J. Phys. A* **23** 4581-4588

[3] Brydges D C and Imbrie J Z 2001 Branched polymers and dimensional reduction *preprint math-ph/0107005*

[4] Cardy J L 1994 Mean area of self-avoiding loops *Phys. Rev. Lett.* **72** 1580-1583 *cond-mat/9310013*

[5] Cardy J L 2001 Exact scaling functions for self-avoiding loops and branched polymers *J. Phys. A* **34** L665-L672 *cond-mat/0107223*

[6] Cardy J L 2002 Conformal invariance in percolation, self-avoiding walks and related problems *preprint cond-mat/0209638*, this volume

[7] Cardy J L and Ziff R M 2002 Exact results for the universal area distribution of clusters in percolation, Ising and Potts models *preprint cond-mat/0205404*

[8] Cardy J L and Guttmann A J 1993 Universal amplitude combinations for self-avoiding walks, polygons and trails *J. Phys. A* **26** 2485-2494 *cond-mat/9303035*

[9] Duchon P 1999 q-Grammars and wall polyominoes *Ann. Comb.* **3** (1999) 311-321

[10] Enting I G and Guttmann A J 1989 Polygons on the honeycomb lattice *J. Phys. A* **22** 1371-1384

[11] Fisher M E Guttmann A J and Whittington S G 1991 Two-dimensional lattice vesicles and polygons *J. Phys. A* **24** 3095-3106

[12] Guttmann A J 1989 Asymptotic analysis of power-series expansions in *Phase Transitions and Critical Phenomena* vol. 13 eds. C Domb and J L Lebowitz (New York: Academic) pp. 1-234

[13] Janse van Rensburg E J 2000 *The Statistical Mechanics of Interacting walks, Polygons, Animals and Vesicles* (New York: Oxford University Press)

[14] Jensen I 2000 Size and area of square lattice polygons *J. Phys. A* **33** 3533-3543 *cond-mat/0003442*

[15] Jensen I 2003 A parallel algorithm for the enumeration of self-avoiding polygons on the square lattice submitted to *J. Phys. A* **36**

[16] Jensen I 2003 Polygons on the hexagonal and triangular lattices in preparation

[17] Jensen I and Guttmann A J 1999 Self-avoiding polygons on the square lattice *J. Phys. A* **32** 4867-4876 *cond-mat/9905291*

[18] Lawler G F Schramm O and Werner W 2002 On the scaling limit of planar self-avoiding walk *preprint math.PR/0204277*

[19] Lawler G F Schramm O and Werner W 2001 Values of Brownian intersection exponents I: Half-plane exponents *Acta Math.* **187** 237-273

[20] Leibler S Singh R R P and Fisher M E 1987 Thermodynamic behaviour of two-dimensional vesicles *Phys. Rev. Lett.* **59** 1989-1992

[21] Louchard G 1984 The Brownian excursion area: a numerical analysis *Comput. Math. Appl.* **10** 413-417

[22] Madras N Orlitsky A and Shepp L A 1990 Monte Carlo Generation of self-avoiding walks with fixed endpoints and fixed length *J. Stat. Phys* **58** 159-183

[23] Madras N and Slade G 1993 *The Self-Avoiding Walk* (Boston, Birkhäuser)

[24] Mandelbrot B 1983 *The Fractal Geometry of Nature* (New York: Freeman)

[25] Nienhuis B 1982 Exact critical point and critical exponents of O(n) models in two dimensions *Phys. Rev. Lett.* **49** 1062-1065

[26] Olver F W J 1958 Uniform asymptotic expansions of solutions of linear second order differential equations for large values of a parameter *Philos. Trans. Roy. Soc. London A* **250** 479-517

[27] Owczarek A L Prellberg T and Brak R 1993 The tricritical behaviour of self-interacting partially directed walks *J. Stat. Phys.* **72** 737-772

[28] Prellberg T 1995 Uniform q-series asymptotics for staircase polygons *J. Phys. A* **28** 1289-1304

[29] Prellberg T and Brak R 1995 Critical exponents from nonlinear functional equations for partially directed cluster models *J. Stat. Phys.* **78** 701-730

[30] Prellberg T and Owczarek R 1995 Stacking models of vesicles and compact clusters *J. Stat. Phys.* **80** 755-779

[31] Prellberg T and Owczarek R 1995 Partially convex lattice vesicles: methods and recent results *Proc. Conf. on Confronting the Infinite* (Singapore: World Scientific) 204-214

[32] Prellberg T and Owczarek A L 1999 On the asymptotics of the finite-perimeter partition function of two-dimensional lattice vesicles *Commun. Math. Phys.* **201** 493-505 *cond-mat/9809156*

[33] Press W H Teukolsky S A Vetterling W T and Flannery B P 1992 *Numerical Recipes in C* (Cambridge: Cambridge University Press) *http://www.nr.com/*

[34] Richard C and Guttmann A J 2001 q-linear approximants: Scaling functions for polygon models *J. Phys. A* **34** 4783-4796 *cond-mat/0109159*

[35] Richard C Guttmann A J and Jensen I 2001 Scaling function and universal amplitude combinations for self-avoiding polygons *J. Phys. A* **34** L495-L501 *cond-mat/0107329*

[36] Richard C 2002 Scaling behaviour of two-dimensional polygon models *J. Stat. Phys.* **108** 459-493 *cond-mat/0202339*