

Honeycomb lattice polygons and walks as a test of series analysis techniques

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Abstract. We have calculated long series expansions for self-avoiding walks and polygons on the honeycomb lattice, including series for metric properties such as mean-squared radius of gyration as well as series for moments of the area-distribution for polygons. Analysis of the series yields accurate estimates for the connective constant, critical exponents and amplitudes of honeycomb self-avoiding walks and polygons. The results from the numerical analysis agree to a high degree of accuracy with theoretical predictions for these quantities.

1. Introduction

Self-avoiding walks (SAWs) and polygons (SAPs) on regular lattices are among the most important and classic combinatorial problems in statistical mechanics. SAWs are often considered in the context of lattice models of polymers while SAPs are used to model vesicles. The fundamental problem is the calculation (up to translation) of the number of SAWs, c_n , with n steps (SAPs, p_n , of perimeter n). As for many interesting combinatorial problems, SAWs have exponential growth, $c_n \sim A\mu^n n^{\gamma-1}$, where μ is the connective constant, γ is a critical exponent, and A is a critical amplitude. A major challenge (short of an exact solution) is the calculation, or at least accurate estimation of, μ , critical exponents and amplitudes. Here our focus is on the numerical estimation of such quantities from exact enumeration data.

The success of series expansions as a numerical technique has relied crucially on several of Tony Guttmann's contributions to the field a asymptotic series analysis. In pioneering the method of differential approximants (see [1] for a review and 'historical notes') Tony Guttmann has given us an invaluable tool which over the years has been proved to be by far the best (in terms both of accuracy and versatility) method for analysing series. In this paper we use long series expansions for self-avoiding polygons and walks on the honeycomb lattice to test the accuracy of various methods for series analysis. For the honeycomb lattice the connective constant, critical exponents and many amplitude ratios are known exactly, making it the perfect test-bed for series analysis techniques.

The rest of the paper is organised as follows: In section 2 we give precise definitions of the models and the properties we investigate and summarise a number of exact results. Section 3 contains a very brief introduction to the literature describing the algorithms used for the exact enumerations. In section 4 we give a brief introduction to the numerical technique of differential approximants and then proceed to analyse the SAP and SAW series clearly demonstrating how we can obtain very accurate estimates for the connective constant and critical exponents.

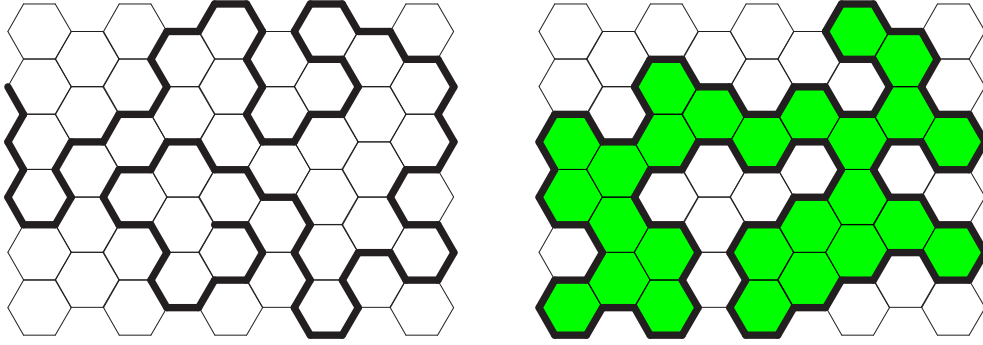


Figure 1. Examples of a self-avoiding walk (left panel) and polygon (right panel) on the honeycomb lattice.

Section 5 is concerned with the estimation of amplitudes. Not only do we obtain very accurate estimates for the amplitudes, but we also show how an analysis of the asymptotic behaviour of the series coefficients can be used to gain insight into corrections to scaling. Finally, in section 6 we discuss and summarise our main results.

2. Definitions and theoretical background

An n -step *self-avoiding walk* ω is a sequence of *distinct* vertices $\omega_0, \omega_1, \dots, \omega_n$ such that each vertex is a nearest neighbour of its predecessor. SAWs are considered distinct up to translations of the starting point ω_0 . We shall use the symbol Ω_n to mean the set of all SAWs of length n . 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 between the two end-points of the walk. The two models are illustrated in figure 1. One is interested in the number of SAWs and SAPs of length n , various metric properties such as the radius of gyration, and for SAPs one can also ask about the area enclosed by the polygon. In this paper we study the following properties:

- (a) the number of n -step self-avoiding walks c_n ;
- (b) the number of n -step self-avoiding polygons p_n ;
- (c) the mean-square end-to-end distance of n -step SAWs $\langle R_e^2 \rangle_n$;
- (d) the mean-square radius of gyration of n -step SAWs $\langle R_g^2 \rangle_n$;
- (e) the mean-square distance of a monomer from the end points of n -step SAWs $\langle R_m^2 \rangle_n$;
- (f) the mean-square radius of gyration of n -step SAPs $\langle R^2 \rangle_n$; and
- (g) the m^{th} moment of the area of n -step SAPs $\langle a^m \rangle_n$.

It is generally believed that the quantities listed above have the asymptotic forms as $n \rightarrow \infty$:

$$c_n = A\mu^n n^{\gamma-1} [1 + o(1)], \quad (1a)$$

$$p_n = B\mu^n n^{\alpha-3} [1 + o(1)], \quad (1b)$$

$$\langle R_e^2 \rangle_n = Cn^{2\nu} [1 + o(1)], \quad (1c)$$

$$\langle R_g^2 \rangle_n = Dn^{2\nu} [1 + o(1)], \quad (1d)$$

$$\langle R_m^2 \rangle_n = En^{2\nu} [1 + o(1)], \quad (1e)$$

$$\langle R^2 \rangle_n = Fn^{2\nu} [1 + o(1)], \quad (1f)$$

$$\langle a^m \rangle_n = G^{(m)} n^{2\nu m} [1 + o(1)]. \quad (1g)$$

The critical exponents are believed to be universal in that they only depend on the dimension of the underlying lattice. The connective constant μ and the critical amplitudes A - $G^{(m)}$ vary from lattice to lattice. In two dimensions the critical exponents $\gamma = 43/32$, $\alpha = 1/2$ and $\nu = 3/4$ have been predicted exactly, though non-rigorously [2, 3]. In this work Nienhuis also predicted the exact value of the connective constant on the honeycomb lattice $\mu = \sqrt{2 + \sqrt{2}}$. When analyzing the series data it is often convenient to use the associated generating functions such as

$$\mathcal{C}(x) = \sum_{n=0} c_n x^n \sim A(x)(1 - \mu x)^{-\gamma}, \quad (2)$$

$$\mathcal{P}(x) = \sum_{n=0} p_{2n+6} x^n \sim B(x)(1 - \mu^2 x)^{2-\alpha}. \quad (3)$$

In the polygon generating function we take into account that SAPs have even length and the smallest one has perimeter 6. The SAW (SAP) generating function has a singularity at the critical point $x = x_c = 1/\mu$ ($x = x_c^2 = 1/\mu^2$) with critical exponent $-\gamma$ ($2 - \alpha$).

The metric properties for SAWs are defined by,

$$\begin{aligned} \langle R_e^2 \rangle_n &= \frac{1}{c_n} \sum_{\Omega_n} (\omega_0 - \omega_n)^2, \\ \langle R_g^2 \rangle_n &= \frac{1}{c_n} \sum_{\Omega_n} \left[\frac{1}{2(n+1)^2} \sum_{i,j=0}^n (\omega_i - \omega_j)^2 \right], \\ \langle R_m^2 \rangle_n &= \frac{1}{c_n} \sum_{\Omega_n} \left[\frac{1}{2(n+1)} \sum_{i=0}^n [(\omega_0 - \omega_j)^2 + (\omega_n - \omega_j)^2] \right], \end{aligned}$$

with a similar definition for the radius of gyration of SAPs.

While the amplitudes are non-universal, there are many universal amplitude combinations. Any ratio of the metric SAW amplitudes, e.g. D/C and E/C , is expected to be universal [4]. Of particular interest is the linear combination [4, 5] (which we shall call the CSCPS relation)

$$H \equiv \left(2 + \frac{y_t}{y_h}\right) \frac{D}{C} - 2 \frac{E}{C} + \frac{1}{2}, \quad (4)$$

where $y_t = 1/\nu$ and $y_h = 1 + \gamma/(2\nu)$. In two dimensions Cardy and Saleur [4] (as corrected by Caracciolo, Pelissetto and Sokal [5]) have predicted, using conformal field theory, that $H = 0$. Cardy and Guttman [6] proved that $BF = \frac{5}{32\pi^2} \sigma a_0$, where σ is an integer constant such that p_n is non-zero when n is divisible by σ , so $\sigma = 2$ for the honeycomb lattice. $a_0 = 3\sqrt{3}/4$ is the area per lattice site on the honeycomb lattice. Richard, Guttman and Jensen [7] conjectured the exact form of the critical scaling function for self-avoiding polygons and consequently showed that the amplitude combinations $G^{(k)} B^{k-1}$ are universal and predicted their exact values. The exact value for $G^{(1)} = \frac{1}{4\pi}$ had previously been predicted by Cardy [8].

The asymptotic form (1a) only explicitly gives the leading contribution. In general one would expect corrections to scaling so

$$c_n = A \mu^n n^{\gamma-1} \left[1 + \frac{a_1}{n} + \frac{a_2}{n^2} + \dots + \frac{b_0}{n^{\Delta_1}} + \frac{b_1}{n^{\Delta_1+1}} + \frac{b_2}{n^{\Delta_1+2}} + \dots \right] \quad (5)$$

In addition to ‘‘analytic’’ corrections to scaling of the form a_k/n^k , where k is an integer, there are ‘‘non-analytic’’ corrections to scaling of the form b_k/n^{Δ_1+k} , where the correction-to-scaling

exponent Δ_1 isn't an integer. In fact one would expect a whole sequence of correction-to-scaling exponents $\Delta_1 < \Delta_2 \dots$, which are both universal and also independent of the observable, that is, the same for c_n, p_n , and so on. Furthermore, there should also be corrections with exponents such as $n\Delta_i + m\Delta_j$, etc., with n and m positive integers. At least two different theoretical predictions have been made for the exact value of the leading non-analytic correction-to-scaling exponent: $\Delta_1 = 3/2$ based on Coulomb-gas arguments [2, 3] and $\Delta_1 = 11/16$ based on conformal-invariance methods [9]. In a recent paper [10] the amplitudes and the correction-to-scaling exponents for SAWs on the square and triangular lattices were studied in great detail. The analysis provided firm numerical evidence that $\Delta_1 = 3/2$ as predicted by Nienhuis.

3. Enumerations

The algorithm we used to enumerate SAPs on the honeycomb lattice is based on the finite-lattice method devised by Enting [11] in his pioneering work, which contains a detailed description of the original approach for enumerating SAPs on the square lattice. A major enhancement, resulting in an exponentially more efficient algorithm, is described in some detail in [12] while details of the changes required to enumerate area-moments and the radius of gyration can be found in [13]. A very efficient parallel implementation is described in [14]. The generalisation to enumerations of SAWs is straight forward as shown in [15]. An implementation of the basic SAP enumeration algorithm on the honeycomb lattice can be found in [16]. Most of the enhancements we made to the square lattice case can also be readily implemented on the honeycomb lattice. The only slightly tricky part is the calculation of metric properties (though the changes are very similar to those required for the triangular lattice [17]).

Using the a parallel version of our honeycomb lattice algorithms we have counted the number of self-avoiding walks and polygons to length 105 and 158, respectively. For self-avoiding walks to length 96 we also calculate series for the metric properties of mean-square end-to-end distance, mean-square radius of gyration and the mean-square distance of a monomer from the end points. In fact the algorithm calculates the metric generating functions with coefficients $c_n \langle R_e^2 \rangle_n$, $n^2 c_n \langle R_g^2 \rangle_n$, and $n c_n \langle R_m^2 \rangle_n$, respectively, the advantage being that these quantities are integer valued. For self-avoiding polygons to length 140 we calculate series for the mean-square radius of gyration and the first 10 moments of the area. Again we actually calculate the series with integer coefficients $8n^2 p_n \langle R^2 \rangle_n$ and $p_n \langle a^k \rangle_n$.

4. Differential approximants

The majority of interesting models in statistical mechanics and combinatorics have generating functions with regular singular points such as those indicated in (2) and (3). The fundamental problem of series analysis is: Given a *finite* number of terms in the series expansion for a function $F(x)$ what can one say about the singular behaviour which after all is a property of the *infinite* series. Without a doubt the best series analysis technique when it comes to locating singularities and estimating the associated critical exponents is differential approximants (see [1] for a comprehensive review of differential approximants and other techniques for series analysis). The basic idea is to approximate the function $F(x)$ by solutions to differential equations with polynomial coefficients. The singular behaviour of such ODEs is much studied (see [18]) and the singular points and exponents are easily calculated.

A K^{th} -order differential approximant (DA) to a function $F(x)$ is formed by matching the coefficients in the polynomials $Q_i(x)$ and $P(x)$ of degree N_i and L , respective, so that (one) of the formal solutions to the inhomogeneous differential equation

$$\sum_{i=0}^K Q_i(x) \left(x \frac{d}{dx}\right)^i \tilde{F}(x) = P(x)$$

Table 1. Critical point and exponent estimates for self-avoiding polygons.

L	Second order DA		Third order DA	
	x_c^2	$2 - \alpha$	x_c^2	$2 - \alpha$
0	0.29289321854(19)	1.50000065(41)	0.29289321865(12)	1.50000040(28)
5	0.29289321875(21)	1.50000010(59)	0.29289321852(48)	1.50000041(99)
10	0.29289321855(23)	1.50000060(48)	0.29289321878(32)	1.49999999(97)
15	0.29289321859(19)	1.50000054(43)	0.29289321861(37)	1.50000035(67)
20	0.29289321866(15)	1.50000038(33)	0.29289321860(21)	1.50000049(43)

agrees with the first $M = L + \sum_i (N_i + 1)$ series coefficients of F . Singularities of $F(x)$ are approximated by the zeros x_i of $Q_K(x)$ and the associated critical exponent λ_i is estimated from the indicial equation. If there is only a single root at x_i this is just

$$\lambda_i = K - 1 - \frac{Q_{K-1}(x_i)}{x_i Q'_K(x_i)}.$$

The physical critical point is the first singularity on the positive real axis.

In order to locate the singularities of the series in a systematic fashion we used the following procedure: We calculate all $[L; N_0, N_1, N_2]$ and $[L; N_0, N_1, N_2, N_3]$ second- and third-order inhomogeneous differential approximants with $|N_i - N_j| \leq 2$, that is the degrees of the polynomials Q_i differ by at most 2. In addition we demand that the total number of terms used by the DA is at least $N_{\max} - 10$, where N_{\max} is the total number of terms available in the series. Each approximant yields N_K possible singularities and associated exponents from the N_K zeroes of $Q_K(x)$ (many of these are of course not actual singularities of the series but merely spurious zeros.) Next these zeroes are sorted into equivalence classes by the criterion that they lie at most a distance 2^k apart. An equivalence class is accepted as a singularity if it appears in more than 75% of the total number of approximants, and an estimate for the singularity and exponent is obtained by averaging over the included approximants (the spread among the approximants is also calculated). The calculation was then repeated for $k - 1, k - 2, \dots$ until a minimal value of 8 was reached. To avoid outputting well-converged singularities at every level, once an equivalence class has been accepted, the data used in the estimate is discarded, and the subsequent analysis is carried out on the remaining data only. One advantage of this method is that spurious outliers, some of which will almost always be present when so many approximants are generated, are discarded systematically and automatically.

4.1. The polygon series

First we apply our differential approximant analysis to the self-avoiding polygon generating function. In table 1 we have listed the estimates for the critical point x_c^2 and exponent $2 - \alpha$ obtained from second- and third-order DAs. We note that all the estimates are in perfect agreement (surely a best case scenario) in that within ‘error-bars’ they take the same value. From this we arrive at the estimate $x_c^2 = 0.2928932186(5)$ and $2 - \alpha = 1.5000004(10)$, where the error-bars reflect the spread among the estimates and the individual error-bars (note that DA estimates *are not* statistically independent so the final error-bars exceed the individual ones). The final estimates are in perfect agreement with the conjectured exact values $x_c^2 = 1/\mu^2 = 1/(2 + \sqrt{2}) = 0.292893218813 \dots$ and $2 - \alpha = 3/2$.

Before proceeding we will consider possible sources of systematic errors. First and foremost the possibility that the estimates might display a systematic drift as the number of terms used is increased and secondly the possibility of numerical errors. The latter possibility is quickly

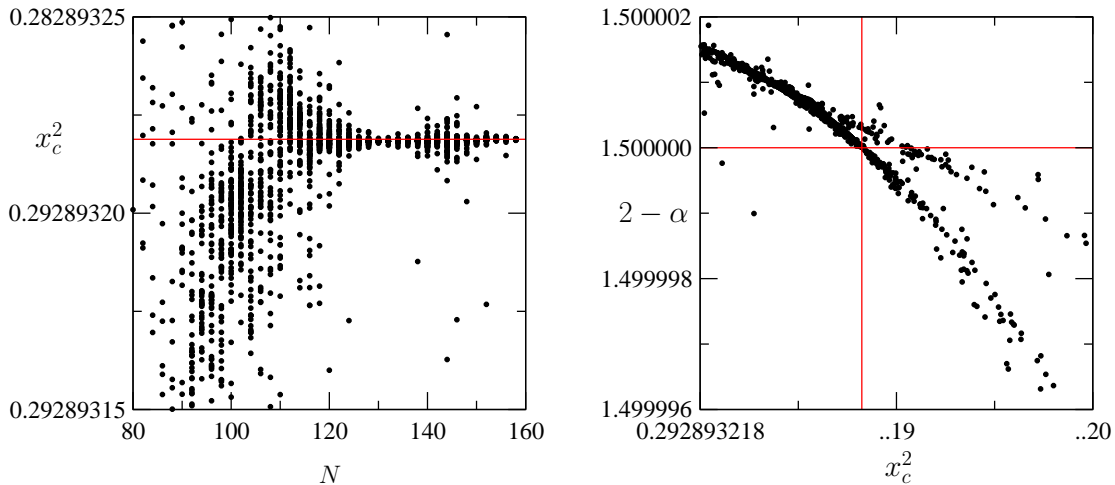


Figure 2. Plot of estimates from third order differential approximants for x_c^2 vs. the highest order term used and $2 - \alpha$ vs. x_c^2 . The straight lines are the exact predictions.

dismissed. The calculations were performed using 128-bit real numbers. The estimates from a few approximants were compared to values obtained using MAPLE with 100 digits accuracy and this clearly showed that the program was numerically stable and rounding errors were negligible. In order to address the possibility of systematic drift and lack of convergence to the true critical values we refer to figure 2 (this is probably not really necessary in this case but we include the analysis here in order to present the general method). In the left panel of figure 2 we have plotted the estimates from third-order DAs for x_c^2 vs. the highest order term N used by the DA. Each dot in the figure is an estimate obtained from a specific approximant. As can be seen the estimates clearly settle down to the conjectured exact value (solid line) as N is increased and there is little to no evidence of any systematic drift at large N . One curious aspect though is the widening of the spread in the estimates around $N = 140$. We have no explanation for this behaviour but it could quite possibly be caused by just a few ‘spurious’ approximants. In the right panel we show the variation in the exponent estimates with the critical point estimates. We notice that the ‘curve’ traced out by the estimates pass through the intersection of the lines given by the exact values. We have not been able to determine the reason for the apparent branching into two parts. However, we note that the lower ‘branch’ contain many more approximants than the upper one.

The differential approximant analysis can also be used to find possible non-physical singularities of the generating function. Averaging over the estimates from the DAs shows that there is an additional non-physical singularity on the negative x -axis at $x = x_- = -1/\mu_-^2 = -0.41230(2)$, where the associated critical exponent α_- has a value consistent with the exact value $\alpha_- = 3/2$. In the left panel of figure 3 we have plotted α_- vs. the highest order term used by the DAs and we clearly see the convergence to a value consistent with $\alpha_- = 3/2$. If we take this value as being exact we can get a refined estimate of x_- from the plot in the right panel of figure 3, where we notice that the estimates for α_- cross the value $3/2$ for $x_- = -0.412305(5)$ which we take as our final estimate. From this we then get $\mu_- = 1.557366(10)$.

4.2. The walk series

Next we apply the differential approximant analysis to the self-avoiding walk generating function. In table 2 we have listed the estimates for the critical point x_c and exponent γ obtained from

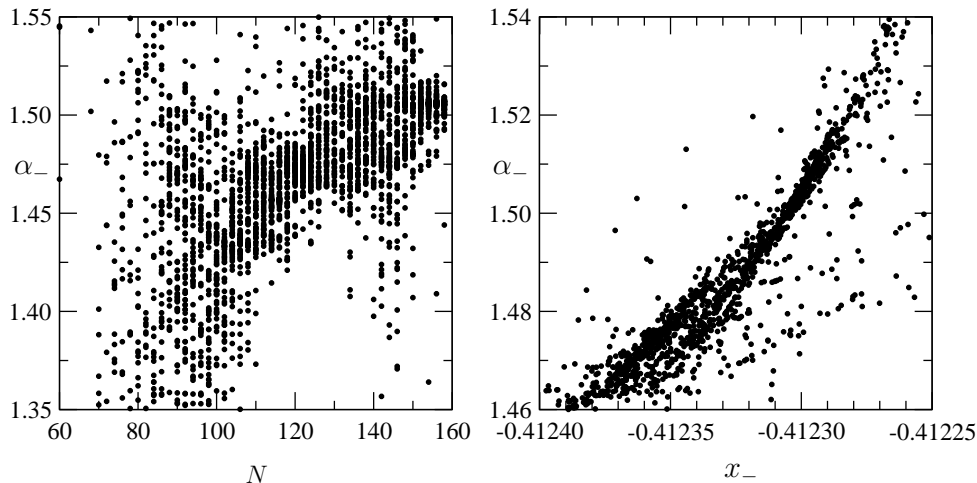


Figure 3. Plot of estimates from third order differential approximants for the location x_- of the non-physical singularity and the associated exponent α_- . The left shows α_- vs. the highest order term used and right panel α_- vs. x_- .

Table 2. Critical point and exponent estimates for self-avoiding walks.

L	Second order DA		Third order DA	
	x_c	γ	x_2	γ
0	0.541196097(19)	1.34360(36)	0.5411961075(19)	1.3437685(54)
5	0.5411961066(10)	1.343770(18)	0.5411961025(10)	1.3437583(19)
10	0.5411961065(12)	1.3437669(53)	0.54119610266(91)	1.3437584(20)
15	0.5411961069(16)	1.343776(68)	0.5411961011(17)	1.3437551(38)
20	0.5411961059(21)	1.3437646(29)	0.5411961022(26)	1.3437580(59)

second- and third-order DAs. Firstly, we note that estimates are about an order of magnitude less accurate than in the polygon case. Secondly, there are now small but nevertheless seemingly systematic differences between the second- and third order DAs (in particular the second-order homogeneous ($L = 0$) approximants are much less accurate than the other cases). On general theoretical grounds one would expect higher-order inhomogeneous approximants to be better in that they can accommodate more complicated functional behaviour. So based mainly on the third-order DAs we finally estimate that $0.541196102(4)$ and $\gamma = 1.343758(8)$. This is consistent with the exact values $x_c = 1/\mu = 1/\sqrt{2 + \sqrt{2}} = 0.541196100146\dots$ and $\gamma = 43/32 = 1.34375$, though the central estimates for γ are systematically a bit too high (and the second-order DAs are worse).

In addition there is a singularity on the negative x -axis at $x = -x_c$ with a critical exponent consistent with the value $1/2$, and a pair of singularities at $x = \pm 0.64215(15)i$ with an exponent which is likely to equal $1/2$ (note that the value $0.64215(15)$ is consistent with $1/\mu_-$). These results help to at least partly explain why the walk series is more difficult to analyse than the polygon series. The walk series has more non-physical singularities and one of these (at $x = -x_c$) is closer to the origin than the non-physical singularity of the polygon series. Furthermore, as argued and confirmed numerically in the next section, the walk series has non-analytical corrections to scaling whereas the polygon series has only analytical corrections. All of these effects conspire to make the walk series much harder to analyse and it is indeed a great testament

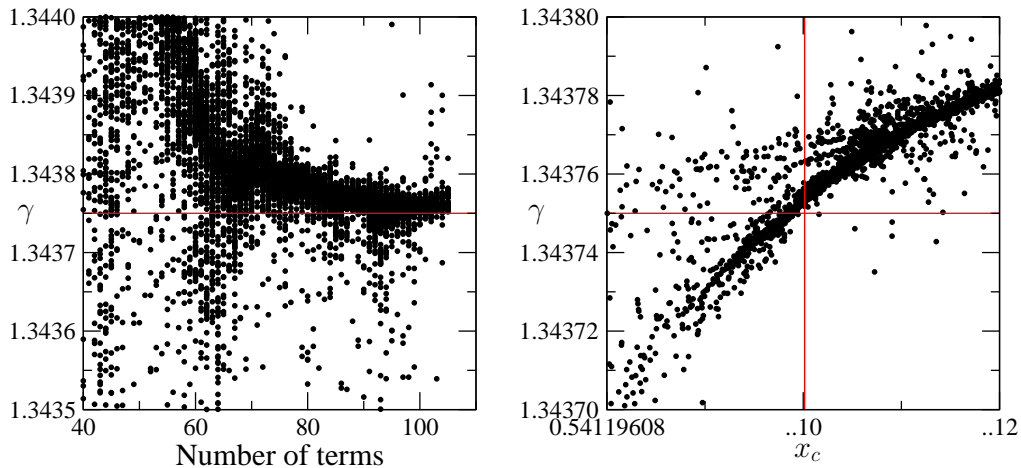


Figure 4. Plot of estimates from third order differential approximants for γ vs. the number of terms used by the DA and γ vs. x_c . The straight lines are the exact predictions.

to the method of differential approximants that the analysis given above yields such accurate estimates despite all these complicating factors.

In figure 4 we have plotted estimates for γ , obtained from third-order DAs, against the number of terms used by the DA (left panel) and against estimates for the critical point x_c (right panel). The estimates for γ display some rather curious and unexpected variations with the number of terms. Early on (around 80 terms) the estimates seem to settle at a value above the exact result. A little later the estimates start trending downwards so that around 95 terms they are in excellent agreement with the exact value. However, the estimates then unexpectedly start trending upwards again so that with more than a 100 terms the agreement with the exact result is only marginal. We also notice that in the right panel estimates for γ vs. x_c happen to just miss the intersection between the lines marking the exact predictions. This behaviour is curious and we have no ready explanation for it other than once again drawing attention to the quite complicated functional form of the generating function. The discrepancies between the estimates and exact values is marginal and certainly not significant enough to raise questions about the correctness of the theoretical predictions.

4.3. Metric properties

Finally, we briefly turn our attention to the series for the metric properties of SAPs and SAWs. We actually study the metric generating functions with integer coefficients $8n^2 p_n \langle R^2 \rangle_n$, $c_n \langle R_c^2 \rangle_n$, $n^2 c_n \langle R_g^2 \rangle_n$, and $n c_n \langle R_m^2 \rangle_n$, which have critical exponents $-(\alpha - 2\nu) = -2$, $-(\gamma + 2\nu) = -91/32 = -2.84375$, $-(\gamma + 2\nu + 2) = -155/32 = -4.84375$, and $-(\gamma + \nu + 1) = -123/32 = -3.84375$, respectively (and as usual the polygon series use only the even terms). In table 3 we list the estimates obtained for the critical point and exponents using averages over third-order DAs. The exponent estimates from the SAP series are consistent with the expected value confirming $\nu = 3/4$ as are the estimates from the SAW series. The only possible exception is the end-to-end distance series where the estimates for both x_c and the exponent are systematically a little too high. However, the discrepancy is not very large and probably not significant.

5. Amplitude estimates

Now that the exact values of μ and the exponents have been confirmed we turn our attention to the “fine structure” of the asymptotic form of the coefficients. In particular we are interested in

Table 3. Critical point and exponent estimates for metric properties of SAPs and SAWs.

L	SAP radius of gyration		SAW end-to-end distance	
	x_c^2	$\alpha + 2\nu$	x_c	$\gamma + 2\nu$
0	0.292893246(10)	2.000176(35)	0.5411961141(14)	2.8438094(28)
5	0.2928932440(70)	2.000169(24)	0.5411961136(31)	2.8438080(64)
10	0.292893245(24)	2.000166(92)	0.5411961124(37)	2.8438054(82)
15	0.292893235(61)	2.00008(27)	0.5411961133(33)	2.8438072(66)
20	0.292893262(42)	2.00019(11)	0.5411961113(25)	2.8438031(59)
L	SAW radius of gyration		SAW distance from end-point	
	x_c	$\gamma + 2\nu + 2$	x_c	$\gamma + \nu + 1$
0	0.541196111(22)	4.843788(47)	0.5411961013(28)	3.8437852(95)
5	0.541196115(12)	4.843806(19)	0.5411961014(21)	3.8437843(90)
10	0.5411961041(91)	4.843789(21)	0.5411961033(52)	3.843789(11)
15	0.5411961021(77)	4.843784(21)	0.5411961064(75)	3.843794(22)
20	0.5411961040(49)	4.843794(10)	0.5411961049(40)	3.8437954(75)

obtaining accurate estimates for the leading critical amplitudes such as A and B . Our method of analysis consists in fitting the coefficients to an assumed asymptotic form. Generally we must include a number of terms in order to account for the behaviour of the generating function at the physical singularity, the non-physical singularities as well as sub-dominant corrections to the leading order behaviour. As we hope to demonstrate, this method of analysis can not only yield accurate amplitude estimates, but it is often possible to clearly demonstrate which corrections to scaling are present.

Before proceeding with the analysis we briefly consider the kind of terms which occur in the generating functions, and how they influence the asymptotic behaviour of the series coefficients. At the most basic level a function $G(x)$ with a power-law singularity

$$G(x) = \sum_n g_n x^n \sim A(x)(1 - \mu x)^{-\xi}, \quad (6)$$

where $A(x)$ is an analytic function at $x = x_c$, gives rise to the asymptotic form of the coefficients

$$g_n \sim \mu^n n^{\xi-1} \left[\tilde{A} + \sum_{i \geq 1} a_i/n^i \right], \quad (7)$$

that is we get a dominant exponential growth given by μ , modified by a sub-dominant term given by the critical exponent followed by analytic corrections. The amplitude \tilde{A} is related to the function $A(x)$ in (6) via the relation $\tilde{A} = A(1/\mu)/\Gamma(\xi)$. If $G(x)$ has a non-analytic correction to scaling such as

$$G(x) = \sum_n g_n x^n \sim (1 - \mu x)^{-\xi} \left[A(x) + B(x)(1 - \mu x)^\Delta \right], \quad (8)$$

we get the more complicated form

$$g_n \sim \mu^n n^{\xi-1} \left[\tilde{A} + \sum_{i \geq 1} a_i/n^i + \sum_{i \geq 0} b_i/n^{\Delta+i} \right]. \quad (9)$$

A singularity on the negative x -axis $\propto (1 + \mu_- x)^{-\eta}$ leads to additional corrections of the form

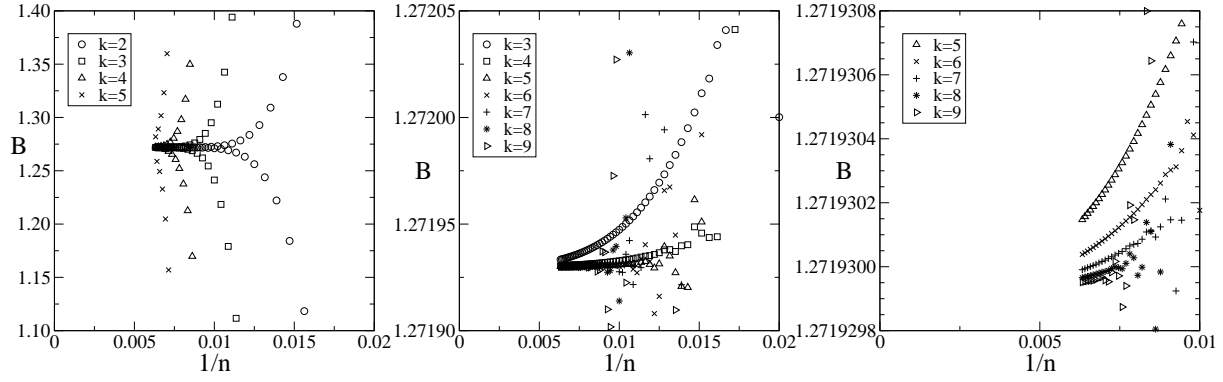


Figure 5. Plots of fits for the self-avoiding polygon amplitude B using in the left panel the asymptotic form (12) which ignores the singularity at $x = x_-$, and in the middle panel the asymptotic form (13) which includes the singularity at $x = x_-$. The right panel gives a closer look at the data from the middle panel.

$$\sim (-1)^n \mu_-^n n^{\eta-1} \sum_{i \geq 0} c_i / n^i. \quad (10)$$

Singularities in the complex plane are more complicated. However, a pair of singularities in the complex axis at $\pm i/\tau$, that is a term of the form $D(x)(1 + \tau^2 x^2)^{-\eta}$, generally results in coefficients that change sign according to a $++--$ pattern. This can be accommodated by terms of the form

$$\sim (-1)^{\lfloor n/2 \rfloor} \tau^n n^{\eta-1} \sum_{i \geq 0} d_i / n^i. \quad (11)$$

All of these possible contribution must then be put together in an assumed asymptotic expansion for the coefficients g_n and we obtain estimates for the unknown amplitudes by directly fitting g_n to the assumed form. That is we take a sub-sequence of terms $\{g_n, g_{n-1}, \dots, g_{n-k}\}$, plug into the assumed form and solve the $k+1$ linear equations to obtain estimates for the first few amplitudes. As we shall demonstrate below this allows us to probe the asymptotic form.

5.1. Estimating the polygon amplitude B

The asymptotic form of the coefficients p_n of the generating function of square and triangular lattice SAPs has been studied in detail previously [19, 12, 14, 17]. There is now clear numerical evidence that the leading correction-to-scaling exponent for SAPs and SAWs is $\Delta_1 = 3/2$, as predicted by Nienhuis [2, 3]. As argued in [19] this leading correction term combined with the $2 - \alpha = 3/2$ term of the SAP generating function produces an *analytic* background term as can be seen from eq. (8). Indeed in the previous analysis of SAPs there was no sign of non-analytic corrections-to-scaling to the generating function (a strong indirect argument that the leading correction-to-scaling exponent must be half-integer valued). At first we ignore the singularity at x_- (since $|x_-| > x_c^2$ it is exponentially suppressed) and obtain estimates for B by fitting p_n to the form

$$p_n = \mu^n n^{-5/2} \left[B + \sum_{i=1}^k a_i / n^i \right]. \quad (12)$$

That is we take a sub-sequence of terms $\{p_n, p_{n-2}, \dots, p_{n-2k}\}$ (n even), plug into the formula above and solve the $k+1$ linear equations to obtain estimates for the amplitudes. It is then

advantageous to plot estimates for the leading amplitude B against $1/n$ for several values of k . The results are plotted in the left panel of figure 5. Obviously the amplitude estimates are not well behaved and display clear parity effects. So clearly we can't just ignore the singularity at x_- (which gives rise to such effects) and we thus try fitting to the more general form

$$p_n = \mu^n n^{-5/2} \left[B + \sum_{i=1}^k a_i/n^i \right] + (-1)^{n/2} \mu_-^n n^{-5/2} \sum_{i=0}^k b_i/n^i. \quad (13)$$

The results from these fits are shown in the middle panel of figure 5. Now we clearly have very well behaved estimates (note the significant change of scale along the y -axis from the left to the middle panel). In the right panel we take a more detailed look at the data and from the plot we estimate that $B = 1.2719299(1)$. We notice that as more and more correction terms are added (k is increased) the plots of the amplitude estimates exhibits less curvature and the slope become less steep. This is very strong evidence that (13) indeed is the correct asymptotic form of p_n .

5.2. Estimating the walk amplitude A

From the differential approximant analysis we found that the walk generating function has non-physical singularities at $x = -x_c$ and $x = \pm i/\mu_-$. In addition we expect from Nienhuis's results (confirmed by extensive numerical work [10]) a non-analytic correction-to-scaling term with exponent $\Delta = 3/2$, and since $\gamma = 43/32$ this correction term does not vanish in the walk case. Ignoring for the moment the pair of complex singularities we first try with to fit to the asymptotic form

$$c_n = \mu^n n^{11/32} \left[A + \sum_{i=2}^k a_i/n^{i/2} \right] + (-1)^n \mu^n n^{-3/2} \sum_{i=0}^k b_i/n^i, \quad (14)$$

where the first sum starts at $i = 2$ because the leading correction is analytic. The resulting estimates for the leading amplitude A are plotted in the top left panel of figure 6. Clearly these amplitude estimates are not well behaved so we better not ignore the complex pair of singularities! Therefore we try again with the asymptotic form

$$c_n = \mu^n n^{11/32} \left[A + \sum_{i=2}^k a_i/n^{i/2} \right] + (-1)^n \mu^n n^{-3/2} \sum_{i=0}^k b_i/n^i + (-1)^{\lfloor n/2 \rfloor} \mu_-^n n^{-3/2} \sum_{i=0}^k c_i/n^i. \quad (15)$$

The estimates for the leading amplitude A are plotted in the top right panel in figure 6. These amplitude estimates are not well behaved either and something is not quite right. Next we try to change the way we included the complex pair of singularities. In (15) we have assumed that all terms arising from the complex singularity have exactly the same sign-pattern. However, if we assume that the analytic correction terms arise from a functional form such as $D(x)(1 + \mu_-^2 x^2)$, where $D(x)$ is analytic, then the analytic correction terms would actually have a *shifted* sign-pattern. We therefore try fitting to the slightly modified asymptotic form

$$c_n = \mu^n n^{11/32} \left[A + \sum_{i=2}^k a_i/n^{i/2} \right] + (-1)^n \mu^n n^{-3/2} \sum_{i=0}^k b_i/n^i + \mu_-^n n^{-3/2} \sum_{i=0}^k (-1)^{\lfloor (n+i)/2 \rfloor} c_i/n^i, \quad (16)$$

where it should be noted that all we have done is change the way we include the terms from the complex singularities so as to shift the sign-pattern by a unit as i is increased. The new estimates for the leading amplitude are plotted in the bottom left panel of figure 6 and quite clearly the convergence is now very much improved. In the bottom right panel of figure 6 we show a much more detailed look at the data and from this plot we can estimate that $A = 1.1449355(5)$.

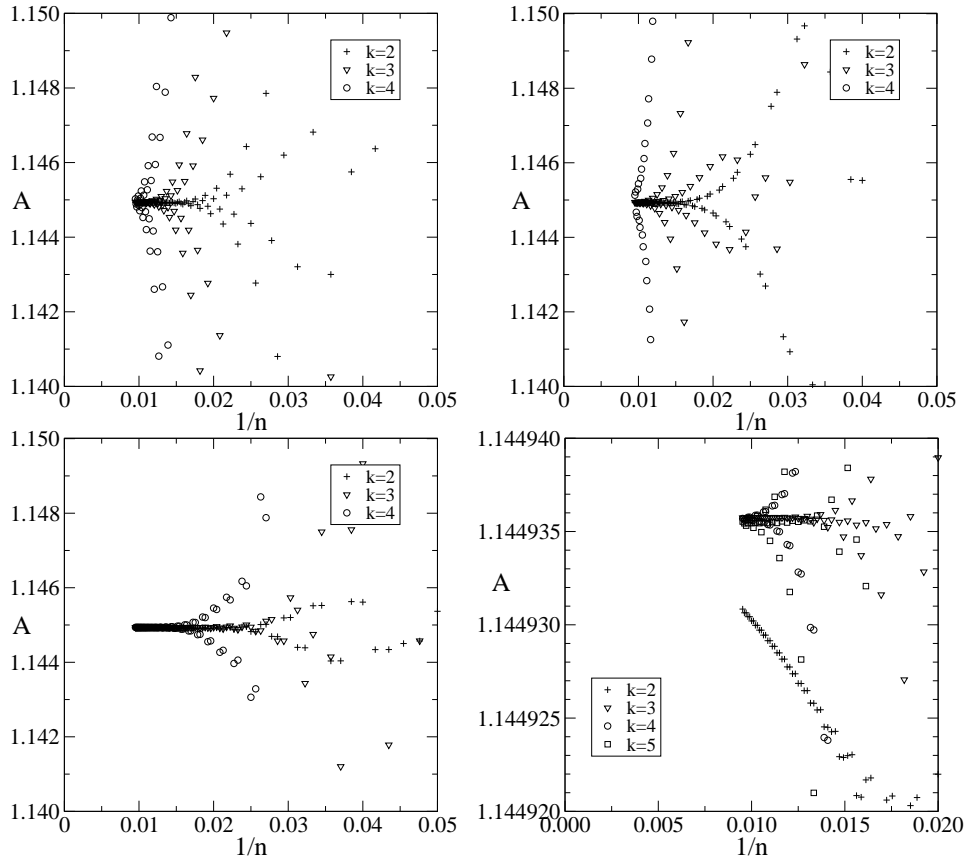


Figure 6. Plots of fits for the self-avoiding walk amplitude A using different asymptotic forms. In the top left panel we show plots using the form (14) which ignores the complex singularity. In the top right panel we include the complex singularity via the form (15) while the bottom left panel includes the complex singularity via the alternative form (16). The bottom right panel is a more detailed look at this latter case.

5.3. The correction-to-scaling exponent

In this section we shall briefly show how the method of direct fitting can be used to differentiate between various possible values for the leading correction-to-scaling exponent Δ_1 (recall the two theoretical prediction $\Delta_1 = 3/2$ by Nienhuis and $\Delta_1 = 11/16$ by Saleur). As already stated there is now firm evidence from previous work that the Nienhuis result is correct. Here we shall present further evidence. Different values for Δ_1 leads to different assumed asymptotic forms for the coefficients. For the SAP series we argued that a value $\Delta_1 = 3/2$ (or indeed any half-integer value) would result only in *analytic* corrections to the generating function and thus that p_n asymptotically would be given by (13). If on the other hand we have a generic value for Δ_1 we would get

$$p_n = \mu^n n^{-5/2} \left[B + \sum_{i=1}^k a_i/n^i + \sum_{i=0}^k b_i/n^{\Delta_1+i} \right] + (-1)^{n/2} \mu^n n^{-5/2} \sum_{i=0}^k c_i/n^i. \quad (17)$$

Fitting to this form we can then estimate the amplitude b_0 of the term $1/n^{\Delta_1}$. We would expect that if we used a manifestly incorrect value for Δ_1 then b_0 should vanish asymptotically thus demonstrating that this term is really absent from (17). So we tried fitting to this form using

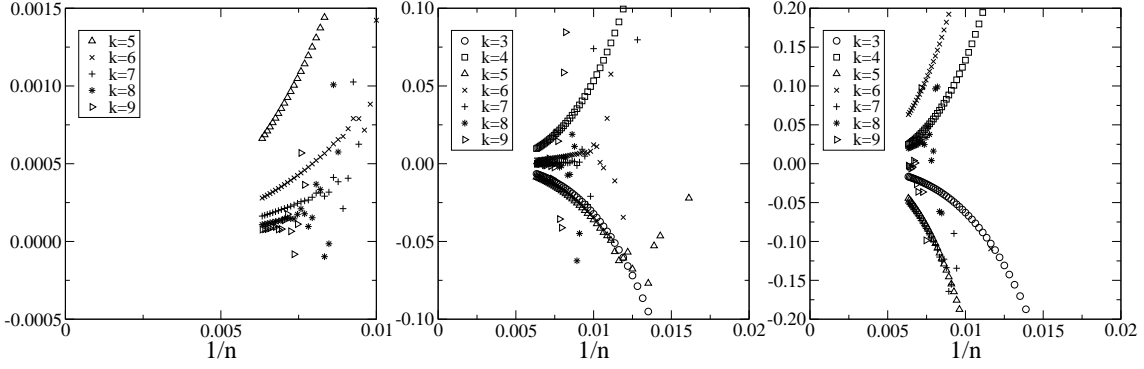


Figure 7. Plots of estimates for the amplitude of the term $1/n^{\Delta_1}$. The left panel shows results from fits to the form (18) where only the leading order term $1/n^{\Delta_1}$ is included (as well as analytical corrections). In the middle panel additional terms of the form $1/n^{\Delta_1+i}$ are included and in the right panel terms like $1/n^{m\Delta_1+i}$ are included.

the value $\Delta_1 = 11/16$. More precisely we fit to the generic form

$$p_n = \mu^n n^{-5/2} \sum_{i=0}^k a_i/n^{\alpha_i} + (-1)^{n/2} \mu_-^n n^{-5/2} \sum_{i=0}^k b_i/n^i. \quad (18)$$

In the first instance we include only the leading term arising from Δ_1 , that is we use the sequence of exponents $\alpha_i = \{0, 11/16, 1, 2, 3, \dots\}$. We also fit to a form in which the additional analytical corrections arising from Δ_1 are included leading to the sequence of exponents $\alpha_i = \{0, 11/16, 1, 27/16, 2, 33/16, 3, 49/16, \dots\}$. As stated in Section 2 more generally one would also expect terms of the form $1/n^{m\Delta_1+i}$ with m a non-negative integer. This leads to fits to the form given above but with $\alpha_i = \{0, 0.6875, 1, 1.375, 1.6875, 2, 2.0625, 2.375, 2.6875, 2.75, 3, \dots\}$. The estimates of the amplitude of the term $1/n^{\Delta_1}$ as obtained from fits to these forms are shown in figure 7. As can be seen from the left panel, where we fit to the first case scenario, the amplitude clearly seems to converge to 0, which would indicate the absence of this term in the asymptotic expansion for p_n . In the middle and right panels we show the results from fits to the more general forms. Again the estimates are consistent with the amplitude being 0. Though in this case the evidence is not quite as convincing. This is however not really surprising given that the incorrect value $\Delta_1 = 11/16$ gives rise to a plethora of absent terms which will tend to greatly obscure the true asymptotic behaviour.

5.4. Amplitude ratios D/C and E/C

From fits to the coefficients in the metric series we find $AC = 1.0141(1)$, $AD = 0.14225(5)$ and $AE = 0.4458(1)$ and thus the ratios are

$$D/C = 0.14027(6) \quad \text{and} \quad E/C = 0.43960(15)$$

D/C and E/C can also be estimated directly from the relevant quotient sequence, e.g. $r_n = \langle R_g^2 \rangle_n / \langle R_e^2 \rangle_n$, using the following method due to Owczarek *et al.* [20]: Given a sequence of the form $g_n \sim g_\infty(1 + b/n + \dots)$, we construct a new sequence $\{h_n\}$ defined by $h_n = \prod_{m=1}^n g_m$. The associated generating function then has the behaviour $\sum h_n x^n \sim (1 - g_\infty x)^{-(1+b)}$, and we can now estimate g_∞ from a differential approximant analysis. In this way, we obtained the estimates

$$D/C = 0.1403001(2) \quad \text{and} \quad E/C = 0.439635(1)$$

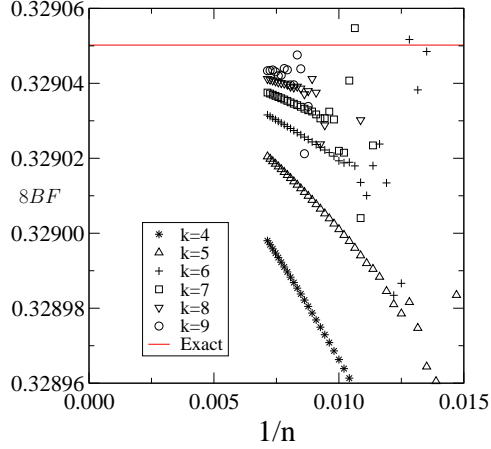


Figure 8. Plots of the estimates for the amplitude combination $8BF$.

These amplitude estimates leads to a high precision confirmation of the CSCPS relation $H = 0.000003(13)$.

5.5. Amplitude combination BF

Next we study the asymptotic form of the coefficients $r_n = 8n^2 p_n \langle R^2 \rangle_n$ for the radius of gyration. The generating function has critical exponent $-(\alpha + 2\nu) = -2$, so the leading correction-to-scaling term no longer becomes part of the analytic background term. We thus use the following asymptotic form:

$$r_n \sim \mu^n n \left[8BF + \sum_{i \geq 0} a_i / n^{1+i/2} \right] + (-1)^{n/2} \mu_-^n n \sum_{i=0}^k b_i / n^i. \quad (19)$$

In figure 8 we plot the resulting estimates for the amplitude $8BF$. The predicted exact value [6] is $BF = \frac{5}{32\pi^2} \sigma a_0 = \frac{15\sqrt{3}}{64\pi^2} = 0.0411312745\dots$, where for the honeycomb lattice $\sigma = 2$ and $a_0 = 3\sqrt{3}/4$. Clearly extrapolation of these numerical results yield estimates consistent with the theoretical prediction.

5.6. Amplitude ratios of area-weighted moments

The amplitudes of the area-weighted moments were studied in [21]. We fitted the coefficients to the assumed form

$$np_n \langle a^m \rangle_n \sim \mu^n n^{2m\nu + \alpha - 2} m! \left[G_m + \sum_{i \geq 0} a_i / n^{1+i/2} \right] + (-1)^{n/2} \mu_-^n n^{2m\nu + \alpha - 2} \sum_{i=0}^k b_i / n^i, \quad (20)$$

where the amplitude $G_m = G^{(m)} B / m!$ is related to the amplitude defined in equation (1g). The scaling function prediction for the amplitudes G_m is [7]

$$G_{2m} B^{2m-1} = -\frac{c_{2m}}{4\pi^{3m}} \frac{(3m-2)!}{(6m-3)!}, \quad G_{2m+1} B^{2m} = \frac{c_{2m+1}}{(3m)! \pi^{3m+1} 2^{6m+2}}, \quad (21)$$

where the numbers c_m are given by the quadratic recursion

$$c_m + (3m-4)c_{m-1} + \frac{1}{2} \sum_{r=1}^{m-1} c_{m-r} c_r = 0, \quad c_0 = 1. \quad (22)$$

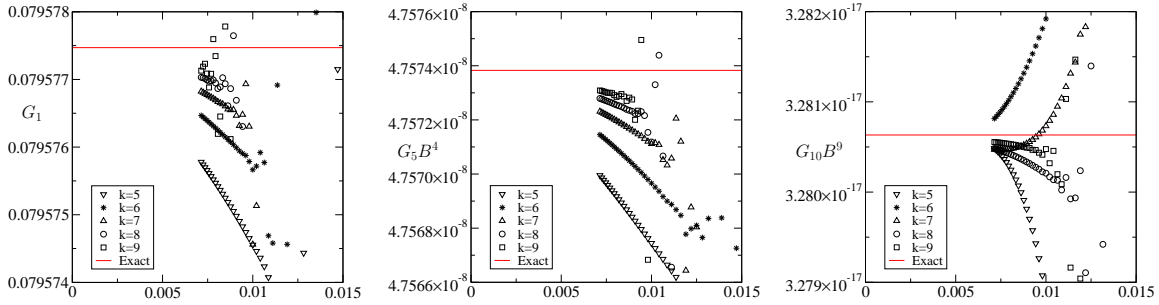


Figure 9. Plots of the estimates for some of the amplitude combinations $G_m B^{m-1}$.

In figure 9 we have plotted the resulting estimates for some of the amplitude ratios. Clearly the numerical results are fully consistent with the theoretical predictions.

6. Summary and conclusions

In this paper we have studied series for self-avoiding walks and polygons on the honeycomb lattice, including series for metric properties and moments of the area-distribution for polygons. We used various methods from Tony Guttmann's tool-kit to analyse the series. The connective constant, critical exponents and many amplitude combinations are known exactly, making it the perfect test-bed for series analysis techniques.

In section 4 we used differential approximants to obtain estimates for the singularities and exponents of the SAP and SAW generating functions. Analysis of the SAP series (section 4.1) yielded very accurate estimates for the critical point $x_c^2 = 0.2928932186(5)$ and exponent $2 - \alpha = 1.5000004(10)$. The estimates agree with the conjectured exact values $x_c^2 = 1/(2 + \sqrt{2}) = 0.292893218813\dots$ and $2 - \alpha = 3/2$. In addition we found clear evidence of a non-physical singularity on the negative axis at $x = x_- = -0.412305(5)$ with an associated critical exponent $\alpha_- = 3/2$. The analysis of the SAW series (section 4.2) also yielded estimates consistent with the predictions of the exact values. In this case there was a non-physical singularity at $x = -x_c$ as well as a pair of complex singularities at $x = \pm 0.64215(15)i$. So the excellent agreement is particularly impressive in light of the quite complicated functional form of the generating function which has at least three non-physical singularities as well as non-analytical corrections to scaling. So the walk series is obviously much harder to analyse and it is a great testament to the method of differential approximants that the analysis nevertheless yields such accurate estimates.

In section 5 we looked closer at the asymptotic form of the coefficients. In particular we obtained accurate estimates for the leading critical amplitudes A and B . Our method of analysis consisted in fitting the coefficients to an assumed asymptotic form. In section 5.1 we analysed the SAP series and demonstrated clearly that in fitting to the coefficients we cannot ignore the singularity at $x = x_-$ even though it is exponentially suppressed asymptotically. After inclusion of this term estimates for the leading amplitude B were well behaved when including only analytic corrections and we found $B = 1.2719299(1)$. We argued that this behaviour was consistent with a corrections-to-scaling exponent Δ_1 being half-integer valued and in particular consistent with the prediction by Nienhuis that $\Delta_1 = 3/2$ (in section 5.3 we showed the absence of a term with $\Delta_1 = 11/16$). In the analysis of the SAW series we discovered some subtleties regarding the inclusion of the terms arising from the complex pair of singularities. Despite a quite complicated asymptotic form (16) taking into account all the singularities and the corrections-to-scaling exponent $\Delta_1 = 3/2$ we could still obtain a quite accurate amplitude estimate $A = 1.1449355(5)$. This analysis clearly shows that it is possible to probe quite deeply

into the asymptotic behaviour of the series coefficients and in particular to distinguish between different corrections to scaling.

E-mail or WWW retrieval of series

The series for the generating functions studied in this paper can be obtained via e-mail by sending a request to I.Jensen@ms.unimelb.edu.au or via the world wide web on the URL <http://www.ms.unimelb.edu.au/~iwan/> by following the instructions.

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