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 [1]. 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, \( c_n \sim A \mu^n n^{-\gamma} \), where \( \mu \) is the connective constant, \( \gamma \) 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, \( \mu \), 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 Guttman’s contributions to the field of asymptotic series analysis. In pioneering the method of differential approximants (see [2] for a review and ‘historical notes’) Tony Guttman 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. 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 \( \omega \) is a sequence of distinct vertices \( \omega_0, \omega_1, \ldots, \omega_n \) such that each vertex is a nearest neighbour of its predecessor. SAWs are considered distinct up to translations of the starting point \( \omega_0 \). We shall use the symbol \( \Omega_n \) to mean the set of all \( n \)-step SAWs. A self-avoiding polygon of length \( n \) is an \( n-1 \)-step SAW such that \( \omega_0 \) and \( \omega_{n-1} \) are nearest neighbours and a closed loop can be formed by inserting a single additional step between the two end-points of the walk. Polygons having the same vertices are identified so that any polygon is generated by \( 2^n \) distinct SAWs since each of the \( n \) vertices could be the starting point and the walk could proceed in two directions. 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 \( \langle R^2_{e} \rangle_n \);
(d) the mean-square radius of gyration of \( n \)-step SAWs \( \langle R^2_{g} \rangle_n \);
(e) the mean-square distance of a monomer from the end points of \( n \)-step SAWs \( \langle R^2_{m} \rangle_n \);
(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 \( \langle a^m \rangle_n \).

The metric properties for SAWs are defined by,

\[
\langle R^2_{e} \rangle_n = \frac{1}{c_n} \sum_{\Omega_n} (\omega_0 - \omega_n)^2,
\]

\[
\langle R^2_{g} \rangle_n = \frac{1}{c_n} \sum_{\Omega_n} \left[ \frac{1}{2(n + 1)^2} \sum_{i,j=0}^{n} (\omega_i - \omega_j)^2 \right],
\]

\[
\langle R^2_{m} \rangle_n = \frac{1}{c_n} \sum_{\Omega_n} \left[ \frac{1}{2(n + 1)} \sum_{j=0}^{n} \left( (\omega_0 - \omega_j)^2 + (\omega_n - \omega_j)^2 \right) \right],
\]

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

It is generally believed [1] that the quantities listed above have the asymptotic forms as \( n \to \infty \):
of the metric SAW amplitudes, e.g., have been predicted by Cardy [9].

When analyzing the series data it is often convenient to use the associated generating functions such as

\[ C(x) = \sum_{n=0}^{\infty} c_n x^n \sim A(x)(1 - \mu x)^{-\gamma}, \]

\[ P(x) = \sum_{n=0}^{\infty} p_{2n+6} x^n \sim B(x)(1 - \mu^2 x)^{2-\alpha}. \]

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 \( x = x_c = 1/\mu \) (\( x = x^2_c = 1/\mu^2 \)) with critical exponent \(-\gamma (2 - \alpha)\).

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 [5]. Of particular interest is the linear combination [5, 6] (which we shall call the CSCPS relation)

\[ H = 2 + \frac{y_l}{y_h} \frac{D}{C} - 2 \frac{E}{C} + \frac{1}{2}, \]

where \( y_l = 1/\nu \) and \( y_h = 1 + \gamma/(2\nu) \). In two dimensions Cardy and Saleur [5] (as corrected by Caracciolo, Pelissetto and Sokal [6]) have predicted, using conformal field theory, that \( H = 0 \). Cardy and Guttmann [7] proved that \( BF = \frac{3}{32\pi} \sigma a_0 \), where \( \sigma \) is an integer constant such that \( p_n \) is non-zero when \( n \) is divisible by \( \sigma \), so \( \sigma = 2 \) for the honeycomb lattice. \( a_0 = 3\sqrt{3}/4 \) is the area per lattice site on the honeycomb lattice. Richard, Guttmann and Jensen [8] 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 \( \sigma = 1 \) had previously been predicted by Cardy [9].

The asymptotic form (2.1a) only explicitly gives the leading contribution. In general one would expect corrections to scaling so

\[ c_n = A\mu^n n^{\gamma-1} \left[ 1 + \frac{a_1}{n} + \frac{a_2}{n^2} + \ldots + \frac{b_0}{n^{\Delta_1}} + \frac{b_1}{n^{\Delta_1+1}} + \frac{b_2}{n^{\Delta_1+2}} + \ldots \right]. \]

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 \( b_k/n^{\Delta_1+k} \), where the correction-to-scaling exponent \( \Delta_1 \) isn’t an integer. In fact one would expect a whole sequence of correction-to-scaling exponents \( \Delta_1 < \Delta_2 \ldots \), 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 (see [10] and references therein for a more detailed discussion of corrections to scaling). We know of two different theoretical predictions for the exact value of the leading non-analytic correction-to-scaling exponent: $\Delta_1 = 3/2$ based on Coulomb-gas arguments [3, 4] and $\Delta_1 = 11/16$ based on conformal-invariance methods [11]. In [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 [12] 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 [13] while details of the changes required to enumerate area-moments and the radius of gyration can be found in [14]. A very efficient parallel implementation is described in [15]. The generalisation to enumerations of SAWs is straightforward as shown in [16]. An implementation of the basic SAP enumeration algorithm on the honeycomb lattice can be found in [17]. 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 [18]).

Using 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 have calculated 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 $c_n \langle R_e^2 \rangle_n$, $(n + 1)^2 c_n \langle R_g^2 \rangle_n$, and $(n + 1)c_n \langle R_m^2 \rangle_n$, respectively, the advantage being that these quantities are integer valued. For self-avoiding polygons to length 140 we have calculated series for the mean-square radius of gyration and the first 10 moments of the area. Again we actually calculated the series with integer coefficients $8n^2 p_n \langle R_e^2 \rangle_n$ 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 (2.2) and (2.3). 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 [2] 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 [19]) 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 $L$, respectively, so that (one) of the formal solutions to the inhomogeneous differential equation

$$
\sum_{i=0}^{K} Q_i(x)(x - \frac{d}{dx})^i \hat{F}(x) = P(x)
$$

agrees with the first $M = L + \sum_i (N_i + 1)$ series coefficients of $F$. We normalise the DA by setting $Q_K(0) = 1$ thus leaving us with $M$ rather than $M + 1$ unknown coefficients. Singularities of $F(x)$ are approximated by the zeros $x_i$ of $Q_K(x)$ and the associated critical exponent $\lambda_i$ is estimated from the
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) |

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

Indicial equation. If there is only a single root at $x_i$ this is just

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

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 is then repeated for $k-1$, $k-2$, ... 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. Unfortunately, it is not possible to provide rigorous error bounds for differential approximant estimates. In quoting errors we have adopted the following general procedure: On individual estimates typically with a fixed value of $L$ the error is calculated from the spread (basically one standard deviation) among the approximants used in obtaining the estimate. Note that these error bounds should not be viewed as a measure of the true error as they cannot include possible systematic sources of error. The final estimates (and error bounds) take into account the individual estimates and their error bounds. Note that DA estimates are not statistically independent so the final error-bar may exceed the individual ones.

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 $2 - \alpha = 1.5000004(10)$. The final estimates are in perfect agreement with the conjectured exact values $x_c^2 = 1/\mu^2 = 1/(2 + \sqrt{2}) = 0.292893218813...$ 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 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. 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, 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 $x = x_- = -\frac{1}{\mu_-^2} = -0.41230(2)$, where the associated critical exponent $\alpha_-$ has a value consistent with the exact value $\alpha_- = 3/2$. In the left panel of figure 3 we have plotted $\alpha_-$ 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 $\alpha_-$ 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 $\gamma$ obtained from 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
Figure 3. Plot of estimates from third order differential approximants for the location $x_-$ of the non-physical singularity and the associated exponent $\alpha_-$. The left shows $\alpha_-$ vs. the highest order term used and right panel $\alpha_-$ vs. $x_-$.  

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

| $L$ | Second order DA | Third order DA |
|-----|-----------------|----------------|
|     | $x_c$           | $\gamma$       | $x_2$           | $\gamma$       |
| 0   | $0.541196697(19)$ | $1.34360(36)$  | $0.5411961075(19)$ | $1.3437685(54)$ |
| 5   | $0.5411961066(10)$ | $1.343770(18)$ | $0.5411961025(10)$ | $1.3437583(19)$ |
| 10  | $0.5411961065(12)$ | $1.343769(53)$ | $0.54119610266(91)$ | $1.3437584(20)$ |
| 15  | $0.5411961069(16)$ | $1.343776(68)$ | $0.5411961011(17)$ | $1.3437551(38)$ |
| 20  | $0.5411961059(21)$ | $1.343764(29)$ | $0.5411961022(26)$ | $1.3437580(59)$ |

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 $x_c = 1/\mu = 1/\sqrt{2 + \sqrt{2}} = 0.541196100146\ldots$ and $\gamma = 43/32 = 1.34375$, though the central estimates for $\gamma$ 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 $1/\mu_-\ldots$). 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 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 $\gamma$, 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 $\gamma$ display some rather curious and unexpected variations with the number of terms. Early on (around 80 terms) the estimates seems 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 $\gamma$ 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 discrepancy 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 $8n^2 p_n (R^2)_n$, $c_n (R^2_e)_n$, $(n + 1)^2 c_n (R^2_g)_n$, and $(n + 1) c_n (R^2_m)_n$, which have critical exponents $-\left(\alpha - 2\nu\right) = -2$, $-\left(\gamma + 2\nu\right) = -91/32 = -2.84375$, $-\left(\gamma + 2\nu + 2\right) = -155/32 = -4.84375$, and $-\left(\gamma + \nu + 1\right) = -123/32 = -3.84375$, 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 to high. However, the discrepancy is not very large and probably not significant.

5. Amplitude estimates

Now that the exact values of $\mu$ 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 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 nonphysical 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
Table 3. Critical point and exponent estimates for metric properties of SAPs and SAWs.

| $L$ | SAP radius of gyration | SAW end-to-end distance |
|-----|------------------------|-------------------------|
|     | $x_s^c$                | $\alpha + 2\nu$          | $x_e$ | $\gamma + 2\nu$          |
| 0   | 0.292893346(10)        | 2.000176(35)             | 0.5411961141(14) | 2.8438094(28)             |
| 5   | 0.29389332440(70)      | 2.000169(24)             | 0.5411961136(31) | 2.8438080(64)             |
| 10  | 0.2938933245(24)       | 2.000166(92)             | 0.5411961124(37) | 2.8438054(82)             |
| 15  | 0.2938933235(61)       | 2.00008(27)              | 0.5411961133(33) | 2.8438072(66)             |
| 20  | 0.2938933262(42)       | 2.00019(11)              | 0.5411961113(25) | 2.8438054(82)             |

| SAW radius of gyration | SAW distance from end-point |
|------------------------|-----------------------------|
|                        | $x_e$ | $\gamma + 2\nu$ + 2 | $x_e$ | $\gamma + \nu + 1$ |
| 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                     | 0.541196104(1)  | 4.843789(21) | 0.5411961033(52) | 3.843794(11)  |
| 15                     | 0.541196102(1)  | 4.843784(21) | 0.5411961064(75) | 3.843794(22)  |
| 20                     | 0.541196104(0)  | 4.843794(10) | 0.5411961049(40) | 3.8437954(75) |

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

$$G(x) = \sum_n g_n x^n \sim A(x)(1 - \mu x)^{-\xi},$$  \hspace{1cm} (5.1)$$

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

$$g_n \sim \mu^n n^{\xi-1} \left[ \tilde{A} + \sum_{i \geq 1} a_i / n^i \right],$$  \hspace{1cm} (5.2)$$

that is we get a dominant exponential growth given by $\mu$, 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 (5.1) via the relation $\tilde{A} = A(1/\mu)/\Gamma(\xi)$. If $G(x)$ has a non-analytic correction to scaling such as

$$G(x) = \sum_n g_n x^n \sim (1 - \mu x)^{-\xi} \left[ A(x) + B(x)(1 - \mu x)^\Delta \right],$$  \hspace{1cm} (5.3)$$

we get the more complicated form

$$g_n \sim \mu^n n^{\xi-1} \left[ \tilde{A} + \sum_{i \geq 1} a_i / n^i + \sum_{i \geq 0} b_i / n^\Delta i \right].$$  \hspace{1cm} (5.4)$$

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

$$\sim (-1)^n \mu_n n^{\eta-1} \sum_{i \geq 0} c_i / n^i.$$  \hspace{1cm} (5.5)$$

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

$$\sim (-1)^{[n/2]} \tau^n n^{\eta-1} \sum_{i \geq 0} d_i / n^i.$$  \hspace{1cm} (5.6)$$
All of these possible contributions 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 \( \{ g_n, g_{n-1}, \ldots, g_{n-k} \} \), 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 [20, 13, 15, 18]. There is now clear numerical evidence that the leading correction-to-scaling exponent for SAPs and SAWs is $\Delta = 3/2$, as predicted by Nienhuis [3, 4]. As argued in [20] 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. (5.3). 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 $x_\pm$ (since $|x_\pm| > x_c^2$ it is exponentially suppressed) and obtain estimates for $B$ by fitting $p_n$ to the form

$$p_n = \mu n^{-5/2} \left[ B + \sum_{i=1}^k a_i / n^i \right]. \quad (5.7)$$

That is we take a sub-sequence of terms \( \{ p_n, p_{n-2}, \ldots, p_{n-2k} \} \) ($n$ 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 $x_\pm$ (which gives rise to such effects) and we thus try fitting to the more general form

$$p_n = \mu n^{-5/2} \left[ B + \sum_{i=1}^k a_i / n^i \right] + (-1)^{n/2} \mu n^{-5/2} \sum_{i=0}^{k} b_i / n^i. \quad (5.8)$$

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 exhibit less curvature and the slope become less steep. This is very strong evidence that (5.8) 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 $x = \pm 1/\mu_-$. 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

$$c_n = \mu n^{1/32} \left[ A + \sum_{i=2}^{k} a_i / n^{i/2} \right] + (-1)^{n} \mu n^{-3/2} \sum_{i=0}^{k} b_i / n^i, \quad (5.9)$$

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
Figure 5. Plots of fits for the self-avoiding polygon amplitude $B$ using in the left panel the asymptotic form (5.7) which ignores the singularity at $x = x_-$, and in the middle panel the asymptotic form (5.8) which includes the singularity at $x = x_-$. The right panel gives a closer look at the data from the middle panel.

\[
c_n = \mu n^{11/32} \left[ A + \sum_{i=2}^{k} a_i/n^{i/2} \right] + (-1)^n \mu n^{-3/2} \sum_{i=0}^{k} b_i/n^i + (-1)^{\lfloor n/2 \rfloor} \mu n^{-3/2} \sum_{i=0}^{k} c_i/n^i. \tag{5.10}
\]

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 (5.10) 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 $D(x)(1 + \mu_2 x^2)^{-\xi}$, where $D(x)$ is analytic, then the correction terms may have a shifted sign-pattern (loosely speaking we expect this to be the case because terms such as $x^k(1 + \mu_2 x^2)^{-\xi}$ generate a sign-pattern shifted by $k$ units and the correction terms from the full functional form may well inherit this shift). We therefore try fitting to the slightly modified asymptotic form

\[
c_n = \mu n^{11/32} \left[ A + \sum_{i=2}^{k} a_i/n^{i/2} \right] + (-1)^n \mu n^{-3/2} \sum_{i=0}^{k} b_i/n^i + \mu n^{-3/2} \sum_{i=0}^{k} (-1)^{\lfloor (n+i)/2 \rfloor} c_i/n^i, \tag{5.11}
\]

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 $A = 1.1449355(5)$.

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 $\Delta_1$ (recall the two theoretical predictions $\Delta_1 = 3/2$ 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 $\Delta_1$ lead 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
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 (5.9) which ignores the complex singularity. In the top right panel we include the complex singularity via the form (5.10) while the bottom left panel includes the complex singularity via the alternative form (5.11). The bottom right panel is a more detailed look at this latter case.

corrections to the generating function and thus that $p_n$ asymptotically would be given by (5.8). If we have a generic value for $\Delta_1$ we would get

$$p_n = \mu^n n^{-5/2} \left[ B + \sum_{i=1}^{k} \alpha_i/n^i + \sum_{i=0}^{k} b_i/n^{\Delta_1+i} \right] + (-1)^{n/2} \mu^n n^{-5/2} \sum_{i=0}^{k} c_i/n^i.$$  (5.12)

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 $\Delta_1$ then $b_0$ should vanish asymptotically thus demonstrating that this term is really absent from (5.12). So we tried fitting to this form using the value $\Delta_1 = 11/16$. More precisely we fit to the generic form

$$p_n = \mu^n n^{-5/2} \sum_{i=0}^{k} \alpha_i/n^i + (-1)^{n/2} \mu^n n^{-5/2} \sum_{i=0}^{k} b_i/n^i.$$  (5.13)

First we include only the leading term arising from $\Delta_1$ using the sequence of exponents $\alpha_i = \{0, 11/16, 1, 2, 3, \ldots\}$. Next we fit to a form including additional analytical corrections arising from $\Delta_1$ leading to the sequence of exponents $\alpha_i = \{0, 11/16, 1, 27/16, 2, 33/16, 3, 49/16, \ldots\}$.
In figure 8 we plot the estimates for the amplitude of the term $1/n^\Delta_1$. The left panel shows results from fits to the form (5.13) 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.

As stated in Section 2 more generally also expects terms of the form $1/n^{m\Delta_1+i}$ with $m$ a non-negative integer. This leads to fits to the form above but with $\alpha_i = \{0, 0.6875, 1, 1.375, 1.6875, 2, 2.0625, 2.375, 2.6875, 2.75, 3 \ldots \}$. The estimates of the amplitude of the term $1/n^{\Delta_1}$ 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 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. The estimates are consistent with the amplitude being 0. Though 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 $D/C = 0.14027(6)$ and $E/C = 0.43960(15)$. The amplitude ratios $D/C$ and $E/C$ can also be estimated directly from the relevant quotient sequence, e.g. $r_n = \langle R_n^2 \rangle / \langle R_{n+i}^2 \rangle$, using the following method due to Owczarek et al. [21]: Given a sequence of the form $g_n \sim g_\infty (1 + b/n + \ldots)$, 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 $g_\infty$ from a differential approximant analysis. In this way, we obtained the estimates $D/C = 0.1403001(2)$ and $E/C = 0.439635(1)$, which leads to a high precision confirmation of the CSCPS relation $H = 0.000003(13)$.

5.5. Amplitude combination $BF$

Next we study the coefficients $r_n = 8n^2 p_n \langle R_n^2 \rangle$ 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 asymptotic form:

$$r_n \sim \mu^n n \left[ 8BF + \sum_{i \geq 0} a_i / n^{1+i/2} \right] + (-1)^{n/2} \mu_n \sum_{i=0}^{k} b_i / n^i. \quad (5.14)$$

In figure 8 we plot the estimates for the amplitude $8BF$. The predicted exact value [7] is $BF = \frac{5}{32\pi^2} \sigma a_0 = \frac{15\sqrt{3}}{64\pi^2} = 0.0411312745 \ldots$, where $\sigma = 2$ and $a_0 = 3\sqrt{3}/4$. By inspection it is clear
that the numerical estimates are fully consistent with the theoretical prediction.

5.6. Amplitude ratios of area-weighted moments

The amplitudes of the area-weighted moments were studied in [22]. We fitted the coefficients to the assumed form

\[ np_m(a^m)_n \sim \mu^n n^{2\nu + \alpha - 2m} \left[ G_m + \sum_{i=0}^k a_i / n^{1+i/2} \right] + (-1)^{n/2} \mu^n n^{2\nu + \alpha - 2} \sum_{i=0}^k b_i / n^i, \tag{5.15} \]

where the amplitude \( G_m = G^{(m)} B / m! \) is related to the amplitude defined in equation (2.1g). The scaling function prediction for the amplitudes \( G_m \) is [8]

\[ G_{2m} B^{2m-1} = - \frac{c_{2m}}{4\pi^3} \frac{(3m-2)!}{(6m-3)!}, \quad G_{2m+1} B^{2m} = \frac{c_{2m+1}}{(3m)! \pi^{3m+1}} \frac{2^{6m+2}}{2^{6m+2}}, \tag{5.16} \]

where the numbers \( c_m \) are given by the quadratic recursion

\[ c_m + (3m - 4)c_{m-1} + \frac{1}{2} \sum_{r=1}^{m-1} c_{m-r}c_r = 0, \quad c_0 = 1. \tag{5.17} \]

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 discussion

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 \( 2 - \alpha = 1.5000004(10) \).
Figure 9. Plots of the estimates for some of the amplitude combinations $G_m B^{m-1}$.

The estimates agree with the conjectured exact values $x_c^2 = 1/(2 + \sqrt{2}) = 0.292893218813\ldots$ 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 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 a more philosophical vein we note that the SAP and SAW generating functions are expected not to be D-finite [23] (a function is D-finite if it is the solution to an ordinary differential equation with polynomial coefficients) and thus not expressible globally as a solution to equations of the form used in the DA analysis. However, the analysis of the SAP generating function in particular clearly indicates that this is not a problem numerically. We expect that the major issue here is whether or not the function can be well-represented locally, around the critical points, by a D-finite function. Further to this point we may briefly mention our recent work with Tony Guttmann on three-choice polygons [24] where we found that the generating function is the solution to an 8th order Fuchsian ODE. However, our analysis of the ODE revealed that the behaviour at each of the critical points is much simpler than one would expect and at each singularity the behaviour locally can be represented by ODEs of lower order. Something similar seems to happen with the more complicated SAP and SAW generating functions.

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 $\Delta_1$ 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 $\Delta_1 = 3/16$). 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 (5.11) 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 can be obtained by request from the author or via the world wide web on the URL http://www.ms.unimelb.edu.au/~iwan/ by following the instructions.

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