Algebraic Techniques for Enumerating Self-Avoiding Walks on the Square Lattice

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Abstract. We describe a new algebraic technique for enumerating self-avoiding walks on the rectangular lattice. The computational complexity of enumerating walks of $N$ steps is of order $3^{N/4}$ times a polynomial in $N$, and so the approach is greatly superior to direct counting techniques. We have enumerated walks of up to 39 steps. As a consequence, we are able to accurately estimate the critical point, critical exponent, and critical amplitude.
1. Introduction

Over the years, the enumeration of square lattice self-avoiding walks has become a benchmark, first for computer performance, and more recently for algorithm design. In the early ‘70s, Sykes et al. (1972) obtained 24 terms of the series by using the chain counting theorem. Direct enumeration is probably somewhat faster, but the graphs enumerated for the chain counting theorem (figure-eights, theta graphs, dumbells and polygons) were useful for other problems in the theory of phase transitions, most notably the Ising model. In 1987 Guttmann extended the series by three terms, using direct enumeration, and in 1991 Guttmann and Wang using a dimerisation algorithm obtained two further terms. Subsequently McDonald et al. (1992) obtained a further term, using an extension of dimerisation to trimerisation. Late in 1991, Masand et al. (1992) used a large supercomputer, a CM-2 containing 65536 processors, to extend the series to 34 terms, running for \( \sim 100 \) hours. All these advances came about because of improvements in computer technology (in large part), with relatively small improvements brought about by algorithm design. (Dimerisation or trimerisation saves a factor of around 2 or 3, but does not ameliorate the exponential growth rate of computer time).

The finite-lattice method plus transfer matrices described here allows 35 terms to be obtained on a work station (an IBM 6000/530 with 256MB of memory) in less time than the 65536 processor CM-2 took to obtain 34 terms. Because of memory requirements, it was necessary to move to a larger machine (an IBM 3090/400 with 500MB memory and 2GB of backing storage) to go from 35 to 39 steps. This computer would be capable of extending the series to 43 terms. However that calculation might take up to a month of c.p.u. time, and so has not been pursued. This improvement however is due to the exponential improvement in algorithm design, rather than evolution of computer speed. This is discussed in more detail below.

The method used is based on the method which Enting and Guttmann have used extensively over the past twelve years to enumerate self-avoiding rings on a square lattice, but is significantly more complicated due to requirement for a second stage of processing.

In a series of papers we have reported some significant improvements in the enumeration of self-avoiding rings on the square lattice extending the known series
(Sykes et al., 1972) from 26 steps to 38 steps (Enting, 1980), 46 steps (Enting and Guttmann, 1985) and 56 steps (Guttmann and Enting, 1988). The extension from 38 steps to 56 steps reflects our use of increasingly powerful computing systems and in particular the use of increasingly large amounts of physical and virtual memory. Only minor changes to our programs have been made, primarily to ‘tune’ the procedure to make efficient use of particular computer architectures. We have also generalised our method to enumerate caliper moments of self-avoiding rings on the square lattice (Guttmann and Enting, 1988) and also to enumerate self-avoiding rings on the L and Manhattan lattices (Enting and Guttmann, 1985) and the honeycomb lattice (Enting and Guttmann, 1989). Most recently we have extended the enumeration of triangular lattice polygons to 25 steps (as reported by Enting and Guttmann, 1990) and then to 35 steps (Enting and Guttmann, 1992).

While our techniques have been highly efficient for enumerating self-avoiding rings they are less suitable for enumerating self-avoiding walks. The difficulty is that walks can span a larger lattice than rings because they are not forced to return. A walk of \( L \) steps can span a distance \( L \) while a ring of \( L \) steps can only span a distance of up to \( L/2 \). For walks constrained by a surface our polygon enumeration techniques could be generalised in analogy with our calculation of surface susceptibilities for the square lattice (Enting and Guttmann, 1980).

The present paper presents an algebraic technique for enumerating self-avoiding walks on a rectangular lattice. The basic quantity that we consider is \( C_{mn} \), the number of walks from a given origin with \( n \) steps in the \( \pm x \) directions and \( m \) steps in the \( \pm y \) directions. We consider segments of walks that double back in the \( y \) direction and which can therefore be counted efficiently by transfer matrix techniques. The general enumeration can be expressed as a combination of such irreducible contributions. We further improve the efficiency of the procedure by restricting the range of the index \( n \) to \( n \leq k \) and reconstruct \( C_{mn} \) for \( m + n \leq 2k + 1 \) by using the symmetry relation

\[
C_{mn} = C_{nm}. \quad (1.1)
\]

The layout of the remainder of this paper is as follows. Section 2 describes the way in which the generating function for self-avoiding walks can be constructed from irreducible contributions. Section 3 shows the way in which these irreducible contributions can be constructed from generating functions for walks on strips that
can be determined by algebraic techniques. Section 4 describes the algorithms for determining the requisite generating functions and analyses the computational complexity of the procedure. Section 5 describes our analysis of the singularity structure of the generating function for self-avoiding walks based on the 39 terms that we have obtained.

2. Generating functions for self-avoiding walks

The generating function for self-avoiding walks on the rectangular lattice is

\[ C(u, w) = \sum_{m,n=0}^{\infty} C_{mn} u^m w^n \]  

(2.1)

The enumeration of the coefficients \( C_{mn} \) is restricted to finite order in \( m \) and/or \( n \) and we generally truncate the double series at \( m + n \leq J \). The obvious summation then gives us the number of walks of up to \( J \) steps on the square lattice.

Our enumeration procedure is based on considering projections of walks onto the \( y \) axis to produce the type of diagrams shown in Figure 1. We refer to segments of walks as irreducible if the projection of that segment onto the \( y \) axis has two or more \( y \) bonds in each position. We will also classify irreducible segments by the number of \( y \) bonds that they span. At this point we need to refine the terminology and distinguish between walks which are directed graphs and chains which are not directed. Our aim is to enumerate walks while the transfer matrix techniques generally enumerate chains. The decomposition of walks into irreducible components makes use of both chains and walks. Figure 2 shows the 5 distinct types of irreducible component that we need to consider.

\( P(u, w) \) is the generating function for walks that have no \( y \) bonds. Thus

\[ P(u, w) = 1 + 2u + 2u^2 + 2u^3 ... = (1 + u)/(1 - u) \]  

(2.2)

\( Q(u, w) \) is the generating function for chains that are irreducible and for which neither end-point lies at an extremal \( y \) coordinate. We also consider subdividing such cases according to \( m \), the number of \( y \) bonds spanned by the projection and define \( Q_m(u, w) \) accordingly. The two pertinent results are
\[ Q(u, w) = \sum_{m=2}^{\infty} Q_m(u, w) \quad (2.3) \]

and

\[ Q_m(u, w) = O(w^{2m}) \quad (2.4) \]

Note that from the definition

\[ Q_0 \equiv Q_1 \equiv 0 \quad (2.5) \]

\( R(u, w) \) is the generating function for irreducible chains with both endpoints having the maximal \( y \) coordinate. Again we subdivide these chains according to the number of \( y \) bonds spanned and put

\[ R(u, w) = \sum_{m=1}^{\infty} R_m(u, w) \quad (2.6) \]

\[ R_m(u, w) = O(w^{2m}) \quad (2.7) \]

and arbitrarily define

\[ R_0 \equiv 0 \quad (2.8) \]

\( S(u, w) \) is the generating function for irreducible chains that have precisely one end having the maximal \( y \) coordinate. Again

\[ S(u, w) = \sum_{m=2}^{\infty} S_m(u, w) \quad (2.9) \]

\[ S_m(u, w) = O(w^{2m+1}) \quad (2.10) \]

and from the definition

\[ S_0 \equiv S_1 \equiv 0 \quad (2.11) \]

Finally \( T(u, w) \) is the generating function for irreducible chains in which the two ends have maximal and minimal \( y \) coordinates. We arbitrarily define

\[ T_0 \equiv 0 \quad (2.12) \]
so that

\[ T(u, w) = \sum_{m=1}^{\infty} T_m(u, w) \quad (2.13) \]

\[ T_m(u, w) = O(w^{3m}) \quad (2.14) \]

When constructing the generating functions for walks we combine the irreducible components represented by \( P, Q, R, S \) and \( T \) by linking them with single \( y \) bonds. These each contribute a factor of \( w \) to the generating function \( C(u, w) \). Two single \( y \) bonds that are adjacent in the projection are actually connected by a type \( P \) irreducible component. A chain whose projection is \( k \) consecutive single \( y \) bonds will have a factor of \( P \) at each internal point. Note that the \emph{walk} generating function \( P \) is required because each distinct direction along the \( x \) axis will generate a distinct chain when combined with \( y \) bonds. If we sum these contributions we can consider linking components of types \( R, S \) and \( T \) with chains of one or more \( y \) bonds connecting type \( P \) walks. The generating function for such chains is

\[
U(u, w) = w + wPw + wPwPw... \\
= w/(1 - wP(u, w)) \quad (2.15)
\]

In the same way we can regard the overall chain as consisting of end segments \( P, R \) or \( S \) connected by combinations of “reducible” parts with generating function \( U \) and irreducible parts with generating function \( T \). The generating function for chains connecting irreducible end segments is thus

\[
V(u, w) = U + UTU + UTUTU + \ldots \\
= U/(1 - TU) \\
= w/(1 - w(T + P)) \quad (2.16)
\]

It is now possible to express the self-avoiding walk generating function as

\[
C(u, w) = P(u, w) + 2[Q(u, w) + 2R(u, w) + 2S(u, w) + T(u, w)] \\
+ 2V(u, w)[P(u, w) + 2R(u, w) + S(u, w) + T(u, w)]^2 \quad (2.17)
\]
The structure of expression (2.17) shows that to obtain an expansion in powers of \( w \), it is necessary to obtain \( Q, R, S, \) and \( T \) to the requisite order. If the irreducible generating functions \( Q_m, R_m, S_m \) and \( T_m \) are known for \( m \leq M \) then \( C(u, w) \) will be correct to \( w^{2M+1} \) (the first incorrect term arising from the absences of \( Q_{M+1} \) and \( R_{M+1} \)). The use of the symmetry relations (1.1) will give \( C_{mn} \) for \( m + n \leq 4M + 3 \).

3. Combining generating functions for chains on strips

The transfer matrix techniques described in the next section produce generating functions for sets of walks confined to strips whose \( y \) coordinates are bounded. Subject to these constraints, all chains are counted, not merely irreducible components. Thus there is a need to relate unrestricted generating functions to the restricted generating functions for irreducible components. In our previous enumerations of self-avoiding rings only linear combinations of different classes of graph were involved and so the restricted generating functions were linear combinations of unrestricted generating functions. The present formalism is more complicated because non-linear relations are involved. We begin by considering \( T^*_M(u, w) \), the generating function for chains whose \( y \) coordinates span \( M \) bonds and which have one end at each \( y \) extremum, that is, \( T^*_M \) is the generating function for bridges. The sum over \( M \) is denoted \( T^*(u, w) \).

By considering the appropriate subset of terms from (2.17) we have

\[
T^*(u, w) = T(u, w) + (P(u, w) + T(u, w))^2 V(u, w). \tag{3.1}
\]

While this equation is formally correct, it is unsuitable for relating \( T^* \) to \( T \) because of the fact that while \( T_m \) is of order \( w^{3m} \), \( T^*_m \) is of order \( w^m \). Thus to obtain \( T \) correct to \( w^K \) would require the calculation of \( T^*_m \) for \( m \leq K \). This difficulty is avoided by introducing an extra variable \( z \) whose power corresponds to the width of the segment under consideration. We refer to functions including \( z \) as “extended generating functions”. We define the extended generating function for irreducible bridges as

\[
X(u, w, z) = P(u, w) + \sum_{m=1}^{\infty} z^m T_m(u, w) \tag{3.2a}
\]
and the extended generating function for all bridges as

\[ X^*(u, w, z) = P(u, w) + \sum_{m=1}^{\infty} z^m T_m^*(u, w) \] (3.2b)

In these terms, \( V(u, w) \), the generating function for bridges ending in single bonds, generalises to

\[ \tilde{V}(u, w, z) = X(u, w, z) = wz/[1 - wzX(u, w, z)] \] (3.3)

Relation (3.1) generalises to

\[ X^*(u, w, z) = X(u, w, z) + X(u, w, z)^2 \tilde{V}(u, w, z) \] (3.4)

whence

\[ X(u, w, z) = X^*(u, w, z)/[1 + wzX^*(u, w, z)]. \] (3.5)

This relation provides the basis of a suitable truncation. The expansion of (3.5) to order \( z^K \) requires \( T_m^* \) for \( m = 1 \) to \( K \) and will give \( T_m \) for \( m = 1 \) to \( K \). The result, noted above, that \( T_m \) is of order \( w^{3m} \) provides a useful check on the algebra.

If we define \( R_m^*(u, w) \) as the generating function for chains in a strip of width \( m \) such that both ends have the maximal \( y \) coordinate then

\[ R_m^*(u, w) = \frac{1}{2}(P(u, w) - 1) + \sum_{n=1}^{m} R_n(u, w) \] (3.6)

This relation can be easily inverted to give individual \( R_m \). These are needed to define \( R(u, w) \) in (2.17) and also to recover the \( S_m(u, w) \) from \( Y(u, w, z) \) (eqn 3.8a) and the \( Q_m(u, w) \) from \( Z(u, w, z) \) (eqn 3.11)

We define \( S_m^*(u, w) \) as the generating function for chains in a strip of width \( m \) where one end of the chain has the maximal \( y \) coordinate and the other end does not have an extremal \( y \) coordinate. The general relation between the irreducible and unrestricted generating functions is

\[ S^*(u, w) = S(u, w) + [S(u, w) + 2R(u, w)] V(u, w) [P(u, w) + T(u, w)] \] (3.7)

We define the extended generating function for irreducible components with one or both ends at the maximal \( y \) co-ordinate as
\[ Y(u, w, z) = 2 \sum_{m=1}^{\infty} z^m R_m(u, w) + \sum_{m=2}^{\infty} z^m S_m(u, w) \] 

(3.8a)

and the corresponding unrestricted function as

\[ Y^*(u, w, z) = 2 \sum_{m=1}^{\infty} z^m R_m^*(u, w) + \sum_{m=2}^{\infty} z^m S_m^*(u, w) \] 

(3.8b)

Eqn. (3.7) generalises to

\[ Y^*(u, w, z) = Y(u, w, z)[1 + \bar{V}(u, w, z)X(u, w, z)] \] 

(3.9)

or

\[ Y(u, w, z) = Y^*(u, w, z)/[1 + \bar{V}(u, w, z)X(u, w, z)] \] 

(3.10)

from which the \( S_m \) can be recovered once \( R_n \) and \( T_n \) are known for \( n \leq m \).

Finally we consider \( Q_m^* \), the generating function for chains in a strip \( X \) where neither end has an extremal \( y \) coordinate.

We have

\[ Q^*(u, w) = Q(u, w) + [P(u, w) + 2R(u, w)]^2 V(u, w) \] 

(3.11)

Defining

\[ Z(u, w, z) = \sum_{m=2}^{\infty} z^m Q_m(u, w) \] 

(3.12a)

and

\[ Z^*(u, w, z) = \sum_{m=2}^{\infty} z^m Q_m^*(u, w) \] 

(3.12b)

gives

\[ Z(u, w, z) = Z^*(u, w, z) - Y(u, w, t)^2 \bar{V}(u, w, z) \] 

(3.13)
4. Transfer matrix enumeration techniques

The analysis in the previous sections has reduced the problem of enumerating general self-avoiding walks of $4K + 3$ steps to one of enumerating walks confined to strips of width $\leq K$ subject to various constraints. In order to enumerate walks confined to strips we use a transfer matrix technique that generalises the approach that we have used in our earlier enumeration of self-avoiding rings. We draw a cross-section line (with a kink) across the width of a strip of width $K$ so as to cut $K+2$ of the bonds on which steps of chains can occur. We note that if we specify the set of occupied steps then the self-avoidance constraint acts independently to the left and right of the cross-section line. However not all combinations of self-avoiding components from the left and right of the cross-section line combine to give walks. It is necessary to consider the connectivity of the components. This can be done by generalising the technique that we used in our earlier work. We assign to each bond intersected by the cross-section line an index

$$n_i = 0, 1, 2, \text{ or } 3 \quad i = 1 \text{ to } K + 2.$$

Here “0” denotes an empty bond, “1” denotes a step connected to a (uniquely defined) later step, “2” denotes a step connected to a (uniquely defined) earlier step and “3” denotes a step not connected to any other steps intersected by the cross-section line.

If we define

$$A(i, j) = \{k : k \leq j \text{ and } n_k = i\} \quad (4.1)$$

then we require

$$|A(1, j)| \geq |A(2, j)| \quad \text{for all } j \quad (4.2a)$$

$$|A(1, K + 2)| = |A(2, K + 2)| \quad (4.2b)$$

as in the enumeration of self-avoiding rings and

$$|A(3, K + 2)| \leq 2. \quad (4.2c)$$

The numbers of sets of $n_i$ subject to these constraints for various $K$ are given in Table 1. These numbers give the main limitation on the size of walks that can be
obtained because it is necessary to store a partial generating function for the number of walks corresponding to each allowed set of $n_i$. These numbers, $s_k$, are larger than the corresponding vector sizes, $r_k$, used in the enumeration of self-avoiding walks, but only by a factor $\gamma(k)$ which is constrained as

$$1 \leq \gamma(k) \leq \frac{1}{2}(k^2 + 5k + 7)$$

Thus the increase in the $s_k$ is dominated by a $3^{k/4}$ increase as for the $r_k$.

Self-avoiding chains in strips are developed successively by advancing the cross-section line so that one vertex of the lattice passes from the right to the left of the line. Except at the beginning of a column, this corresponds to moving the kink down one row. This move replaces two bonds (and their associated $n_i$) by two new bonds with new $n_i$. The other $n_i$ are unchanged except when the addition of the new site changes the connectivity of the components. Table 2 shows the various combinations of new $n_i$ that can be produced from various combinations of old $n_i$ pairs. Various special cases occur. If a link from a free end (i.e. $n_i = 3$) connects to an existing loop segment then the other end of the loop must be reset to type 3. If two loops meet then one end must be relabelled. The closing of a single loop implies that a ring, disconnected from the walk, has been created and this configuration is ignored. The final step in the construction of a chain is when two type 3 bonds meet. When this occurs, all other bonds must be empty for a valid chain generating function to be added to the running total. If this is not the case it implies that other disconnected components are present and the configuration is ignored.

The iteration is initiated from an empty state ($n_i \equiv 0$) with generating function 1. As each bond is added, factors of $v$ or $w$ as appropriate are used to multiply the old partial generating function and the product is accumulated into the running total for the new partial generating function. Each chain could, in principle, be generated for a number of different $x$ and $y$ displacements from a given reference origin. To ensure uniqueness in the $x$ direction, the chain is required to intersect the first column considered. Thus the state with all $n_i$ zero is never continued after the first column has been built up. This ensures that each chain is counted only once and, together with the requirement that the last operation is to join two type 3 bonds, also ensures that only one connected component occurs in each graph that is counted. Formally, if $4k+3$ series terms are required then the transfer matrix operation must be
repeated until $4k + 3$ columns of each strip have been generated. This will ensure that all the cancellations involved in going from unrestricted to irreducible contributions will be correct. As noted above, the cancellations provide a useful check on the implementation of the algebraic formalism. If however the check is not required then the results (2.4), (2.7), (2.10) and (2.14) can be assumed to be true. For a strip of width $M$ it is sufficient to generate only $4k + 3 - 2M$ columns of the strip.

This requires a large amount of memory to store all the intermediate generating functions. If this amount of memory is not available as physical memory, but only as virtual (disk based) memory, the performance can be enhanced greatly by being careful of the order in which the partial generating functions are processed. This can make the entire process close to sequential, and enormously reduce the amount of disk access required.

As mentioned before, when a partial generating function is processed, only the two $n_i$ coefficients adjacent to the site being added will change, unless this changes the connectivity of a loop. However in this case, it will always be a non-zero going to another non-zero, so if we make up a “partial signature” out of the $n_i$ coefficients that are not being directly changed, and just record whether they are zero or not, this partial signature will be invariant under the transfer matrix. That is, all “new” partial generating functions will have the same “partial signature”.

We can then process all the partial generating functions with one particular partial signature, save the results to disk, and process the next set, until all are processed. We do not need to worry about the possibility of having to accumulate a new partial generating function to one stored on disk, as if two partial generating functions have different partial signatures, they definitely cannot have the same “full signature” ($n_i$ values).

The only problem with this is to make sure that we process all the partial generating functions of a particular partial signature first. Fortunately, one can get away without having to sort the output file before using it as input. If instead of saving to just one output file, two output files are used, it is possible to arrange things such that one only has to read from these two files in order, and the data will be ordered in exactly the right way for adding the next site. This minimises the amount of disk access. To obtain this nice ordering, one looks at whether the new value of $n_i$ which will be included in the partial signature for the next phase is zero.
or not, and accordingly assigns it to one of the two output files. This will arrange the partial signatures in binary order, with the most significant bit in the partial signature being the most recent bit calculated, and the least significant bit being the oldest bit calculated.

This method has a side benefit — in a multi-processor architecture, one can have each processor working independently on separate partial signature groups, with very little inter-processor communication. This means that this algorithm is easy to parallelise, which will become increasingly important in the future as parallel computers are becoming more and more popular, whilst many algorithms are difficult to parallelise.

The problem of ensuring uniqueness in the $y$-direction requires inclusion-exclusion arguments of the type used in our enumeration of self-avoiding rings. For a strip of width $M$ we classify chain generating functions as $G_m(\pm, \pm, \pm)$ where $+$ denotes an allowed location for ends and $-$ denotes a forbidden location. The three arguments refer to the top row, the bottom row and the set of internal rows respectively. Specifying the end locations permissively, rather than prescribing how many end points lie in each set allows us to treat the two ends of the chain independently. We have

$$G_K(+, -, -) = \frac{P - 1}{2} + \sum_{m=1}^{K} R_m$$  (4.3a)

$$G_K(+, +, -) = T^K_K + P - 1 + 2 \sum_{m=1}^{K} R_m$$  (4.3b)

$$G_K(+, -, +) = K \left(\frac{P - 1}{2}\right) + \sum_{m=1}^{K} (K + 1 - m)(R_m + Q^K_m + S^K_m)$$

$$+ \sum_{m=1}^{K} (K - m)(T^K_m + R_m + S^K_m)$$  (4.3c)

$$G_K(-, -, +) = (K - 1) \left(\frac{P - 1}{2}\right) + \sum_{m=1}^{K} (K + 1 - m)Q^K_m + 2 \sum_{m=1}^{K-1} (K - m)(R_m + S^K_m)$$

$$+ \sum_{m=1}^{K-2} (K - 1 - m)T^K_m$$  (4.3d)

These relations can be explicitly inverted to give
\[ R_m = G_m(+, -, -) - G_{m-1}(+, -, -) \] (4.4a)

\[ Q_m^* = G_m(-, -, +) - G_{m-1}(+, +, +) - \sum_{n=1}^{m-1} (Q_n^* + R_n + S_n^*) \] (4.4b)

\[ S_m^* = G_m(+, -, +) - G_{m-1}(+, -, +) - G_m(+, -, -) - G_{m-1}(+, -, -) \]

\[-\frac{P-1}{2} - Q_m^* - \sum_{n=1}^{m-1} (Q_n^* + 2S_n^* + T_m^*) \] (4.4c)

\[ T_m^* = G_m(+, +, -) - 2G_m(+, -, -) \] (4.4d)

5. Analysis of series

This algorithm was implemented for computers in two parts. The first part was the transfer matrix portion; that is, it computed the $G$ functions. This was the time and memory intensive section. It was run up to a width of 8 on an IBM RS6000/520 with 256MB or RAM, then to width 9 on an IBM 3090 with 500MB RAM and 2GB backing store. It required about 200MB and 600MB of memory respectively, and required several days in each case. The same machine could have been used to do width 10 (43 terms) given several weeks of processor time. This program was written in C, and reused memory whenever possible (there was only one bank of memory, used for both the about-to-be-processed partial generating functions, and the have-just-been-processed partial generating functions). The method described previously for using disk storage efficiently was implemented and tested, but not used as whilst memory was then no longer a problem, time became a large problem.

The second part performed all the algebra. Whilst algebra on large (over 15000 coefficients) polynomials in three variables is slow, it is still a minor problem compared to the transfer matrix section, requiring time in only hours and memory in sub-megabytes, so efficiency was not as vital. It was implemented in C++.

The results for width 9 (39 terms) are given in table 3.

The method of analysis used is based on first and second order differential approximants. It was also used in previous papers [Guttmann (1987), Guttmann and
Wang (1989) and is described in detail in Guttmann (1989)]. In summary, we construct near-diagonal inhomogeneous approximants, with the degree of the inhomogeneous polynomial increasing from 1 to 8 in steps of 1. For first order approximants (K=1), 12 approximants are constructed that utilise a given number of series coefficients, N. Rejecting occasional defective approximants, we form the mean of the estimates of the critical point and critical exponent for fixed order of the series, N. The error is assumed to be two standard deviations. A simple statistical procedure combines the estimates for different values of N by weighting them according to the error, with the estimate with the smallest error having the greatest weight. As the error tends to decrease with the number of terms used in the approximant, this procedure effectively weights approximants derived from a larger number of terms more heavily.

For second order approximants (K=2), we construct 8 distinct approximants for each value of N. A summary of the results of this process is shown in Table 4. The statistical procedure used to combine the results gives

\[ x_c = 0.379052 \pm 0.000001 \quad \gamma = 1.3435 \pm 0.0003 \quad (K = 1) \]

\[ x_c = 0.3790520 \pm 0.0000005 \quad \gamma = 1.3436 \pm 0.00015 \quad (K = 2) \]

These results provide abundant support, if support is still needed, for the value \( \gamma = 1.34375 \) obtained by Nienhuis (1982, 1984). To refine the estimate of the critical point, linear regression is used. There is a strong correlation between estimates of the critical point and critical exponent. This is quantified by linear regression, and in this way the biased estimates (biased at \( \gamma = 43/32 \)) are obtained.

We find

\[ x_c = 0.3790524 \pm 0.0000005 \quad (K = 1) \]

\[ x_c = 0.3790525 \pm 0.0000005 \quad (K = 2) \]

These are in excellent agreement with previous estimates based on the 56 term polygon series (Guttmann and Enting, 1988), \( x_c = 0.37905228 \pm 0.00000014 \)

For the honeycomb lattice, the “connective constant” = 1/\( x_c \) is known exactly (Nienhuis 1982, 1984), and is \( \sqrt{2 + \sqrt{2}} \), which satisfies a simple quadratic equation in \( x_c^2 \). A feature of Maple (Version 5) is a clever algorithm for seeking polynomials with integer coefficients that have a given root. Attempting to find a quartic polynomial
that gave as a root the biased value of $x_c$ quoted above, we found the best solution was also a polynomial quadratic in $x_c^2$. It was

$$581x^4 + 7x^2 - 13 = 0.$$  

The root is $x_c = 0.37905227...$. While we consider it would be fortuitous if this were the true value of the critical point, it nevertheless provides a useful mnemonic.

Another analysis we were able to carry out with this long series was a study of amplitudes of the leading term and the correction terms. As previously discussed for self-avoiding polygons (Guttmann and Enting 1988), we have found no evidence for any non-analytic correction-to-scaling term other than that suggested by Nienhuis, with a “correction” exponent of $\Delta = 1.5$. In the case of the polygon generating function this “folds into” the additive analytic term. However, for the SAW series, it gives rise to a non-analytic correction term. Furthermore, there is another singularity on the negative real axis, at $x = -x_c$, as shown by Guttmann and Whittington (1978).

Thus we expect the generating function for walks to behave like

$$C(x) = \sum c_n x^n \sim A(x)(1-\mu x)^{-43/32}[1+B(x)(1-\mu x)^{3/2}...] + D(x)(1+\mu x)^{-1/2}. \quad (5.1)$$

The exponent for the singularity on the negative real axis reflects the fact that this term is expected to behave as the energy, and hence to have exponent $\alpha - 1$, where $\alpha = \frac{1}{2}$. From the above, it follows that the asymptotic form of the coefficients, $c_n$, behaves like:

$$c_n \sim \mu^n [a_1 n^{11/32} + a_2 n^{-21/32} + b_1 n^{-37/32} + (-1)^n d_1 n^{-3/2} + (-1)^n d_2 n^{-5/2}] \quad (5.2)$$

The five amplitudes, $a_1, a_2, b_1, d_1$ and $d_2$ come from the leading singularity (giving rise to $a_1$ and $a_2$), the correction-to-scaling term (giving rise to $b_1$) and the term on the negative real axis (giving rise to $d_1$ and $d_2$). A small program written in Mathematica was used to fit successive quintuples of coefficients, $c_{n-4}, c_{n-3}, c_{n-2}, c_{n-1}$ and $c_n$ for $n = 6,7,8,...,39$. The results are given in table 5.

With the possible exception of the sequence $\{d_2\}$, the sequences for the various amplitudes appear to be converging. Various other values for the exponents were also tried, including a square-root correction-to-scaling term. In all cases the convergence was dramatically worsened by such changes. Indeed, with a square-root correction-to-scaling exponent, a number of sequences appeared to diverge rather than converge.
However, we have assumed above that the sub-leading term of the singularity on the negative real axis is analytic. If we allow this singularity to be a square root singularity, so that the last term in eqn. (5.2) above becomes \( \mu^n(-1)^n d_2 n^{-2} \) then the results are even better converged, as shown in Table 6.

From these tables we estimate \( a_1 \approx 1.1771, a_2 \approx 0.554, b_1 \approx -0.19, d_1 \approx -0.19, \) where errors are expected to be confined to the last quoted digit in each case. Repeating the above calculations with a critical point shifted by twice the confidence limit quoted does not change these amplitude estimates.

This then completes our numerical study of the generating function for self avoiding walks.

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References

Enting I G , 1980  *J. Phys. A: Math. Gen* 13 3713.
Enting I G and Guttmann A J 1985 *J. Phys. A: Math. Gen.* 18 1007.
— 1989 *J. Phys. A: Math. Gen.* 22 1371
— 1990 *J Stat. Phys.* 58 475
— 1992 *J. Phys. A: Math. Gen.* 25 2791
Guttmann A J, 1987 *J. Phys. A: Math. Gen.* 20 1839
— 1989 In: *Phase Transitions and Critical Phenomena* 13. eds. C. Domb and J. Lebowitz (Academic Press, London)
Guttmann A J and Enting I G , 1988 *J. Phys. A: Math. Gen.* 21 L165
Guttmann A J and Wang J S, 1991 *J. Phys. A: Math. Gen.* 24 3107
Guttmann A J and Whittington S G 1978 *J. Phys. A: Math. Gen.* 11 721
MacDonald D, Hunter D L, Kelly K and Jan N, 1992 *J. Phys. A: Math. Gen.* 25 1429
Masand B, Wilensky U, Maffar J P and Redner S, 1992 *J. Phys. A: Math. Gen.* 25 L365
Nienhuis B, 1982 *Phys. Rev. Lett.* 49 1062
Nienhuis B, 1984 *J. Stat. Phys.* 34 731
Sykes M F and Guttmann A J, Roberts P D and Watts M G 1972 *J. Phys. A: Math. Gen.* 5 653
Tables and table captions

Table 1. The sizes of vectors required by the transfer matrix formalism. For ring enumeration $r_k$ components are required. For walk enumeration $s_k$ components are required.

| Strip width, k | #bonds | $r_k$ | $s_k$ |
|---------------|--------|------|------|
| -             | 1      | 1    | 2    |
| -             | 2      | 2    | 5    |
| 1             | 3      | 4    | 13   |
| 2             | 4      | 9    | 37   |
| 3             | 5      | 21   | 106  |
| 4             | 6      | 51   | 312  |
| 5             | 7      | 127  | 925  |
| 6             | 8      | 323  | 2767 |
| 7             | 9      | 835  | 8314 |
| 8             | 10     | 2188 | 25073|
| 9             | 11     | 5798 | 75791|
| 10            | 12     | 41835| 229495|
Table 2. Allowed transformations of bond indices. For the operations, “Build” means incorporate the contribution into the new vector, as defined by the new indices. “R(a → b)” means apply the change a → b to the other end of the chain in order to specify the index in the new vector. “Ignore” means perform no operation, as a disconnected ring has been generated. “Acc” means accumulate the vector component into the chain generating function if all the other $n_i$ are zero, otherwise the operation preceding the “OR” is applied.

| Old indices $\ (n_j, n_{j+1})$ | New indices $\ (n_j, n_{j+1})$ | Operation          |
|-------------------------------|-------------------------------|--------------------|
| (0,0)                         | (0,0), (0,3), (3,0) or (1,2)  | Build              |
| (0,1) or (1,0)                | (0,1), (1,0) or (0,0)         | R(2 → 3)           |
| (0,2) or (2,0)                | (0,2), (2,0) or (0,0)         | R(1 → 3)           |
| (0,3) or (3,0)                | (0,3), (3,0)                  | Build OR Acc       |
| (1,1)                         | (0,0)                         | R(2 → 1)           |
| (2,2)                         | (0,0)                         | R(1 → 2)           |
| (1,2)                         | -                             | Ignore             |
| (2,1)                         | (0,0)                         |                    |
| (3,3)                         | -                             | Ignore OR Acc      |
| (3,1), (1,3)                 | (0,0)                         | R(2 → 3)           |
| (3,2), (2,3)                 | (0,0)                         | R(1 → 3)           |
Table 3. Numbers of self avoiding walks.

| $n$ | $c_n$ |
|-----|-------|
| 0   | 1     |
| 1   | 4     |
| 2   | 12    |
| 3   | 36    |
| 4   | 100   |
| 5   | 284   |
| 6   | 780   |
| 7   | 2172  |
| 8   | 5916  |
| 9   | 16268 |
| 10  | 44100 |
| 11  | 120292|
| 12  | 324932|
| 13  | 881500|
| 14  | 2374444|
| 15  | 6416596|
| 16  | 17245332|
| 17  | 46466676|
| 18  | 124658732|
| 19  | 335116620|
| 20  | 897697164|
| 21  | 2408806028|
| 22  | 6444560484|
| 23  | 17266613812|
| 24  | 46146397316|
| 25  | 123481354908|
| 26  | 329712786220|
| 27  | 881317491628|
| 28  | 2351378582244|
| 29  | 6279396229332|
| 30  | 16741957935348|
| 31  | 44673816630956|
| 32  | 119034997913020|
| 33  | 317406598267076|
| 34  | 845279074648708|
| 35  | 2252534077759844|
| 36  | 5995740499124412|
| 37  | 15968852281708724|
| 38  | 42486750758210044|
| 39  | 113101676587853932|
Table 4. Estimates of the critical point ($x_c$) and critical exponent ($\gamma$) from first order (K=1) and second order (K=2) differential approximants. $L$ is the number of approximants used. If $L$ is too small (marked with an ‘x’), the estimates are not used in the subsequent statistical analysis.

| $K$ | $n$ | $x_c$       | error    | $\gamma$       | error    | $L$ |
|-----|-----|-------------|----------|----------------|----------|-----|
| 1   | 19  | 0.3790473   | —        | -1.3430184     | —        | 1x  |
| 1   | 20  | 0.3790495   | .000004  | -1.3432502     | .0001073 | 2x  |
| 1   | 21  | 0.3790526   | .000105  | -1.3435231     | .0016130 | 4   |
| 1   | 22  | 0.3790469   | .000133  | -1.3427806     | .0021290 | 4   |
| 1   | 23  | 0.3790468   | .000071  | -1.3427666     | .0011925 | 5   |
| 1   | 24  | 0.3790520   | .000038  | -1.3436373     | .0006432 | 7   |
| 1   | 25  | 0.3790525   | .000052  | -1.3437004     | .0010102 | 9   |
| 1   | 26  | 0.3790508   | .000050  | -1.3433692     | .0010094 | 11  |
| 1   | 27  | 0.3790530   | .000074  | -1.3437617     | .0013817 | 12  |
| 1   | 28  | 0.3790519   | .000016  | -1.3435724     | .0003713 | 12  |
| 1   | 29  | 0.3790519   | .000010  | -1.3435632     | .0002717 | 9   |
| 1   | 30  | 0.3790517   | .000016  | -1.3435091     | .0004340 | 9   |
| 1   | 31  | 0.3790518   | .000011  | -1.3435230     | .0003276 | 8   |
| 1   | 32  | 0.3790514   | .000017  | -1.3434149     | .0005073 | 4   |
| 1   | 33  | 0.3790521   | .000016  | -1.3436098     | .0004159 | 9   |
| 1   | 34  | 0.3790525   | .000028  | -1.3437270     | .0007447 | 11  |
| 1   | 35  | 0.3790518   | .000003  | -1.3435417     | .0000956 | 10  |
| 1   | 36  | 0.3790519   | .000003  | -1.3435722     | .0001233 | 10  |
| 1   | 37  | 0.3790517   | .000011  | -1.3434730     | .0004568 | 8   |
| 1   | 38  | 0.3790518   | .000009  | -1.3435048     | .0003501 | 9   |
| 1   | 39  | 0.3790521   | .000001  | -1.3436392     | .0000515 | 2x  |
| 2   | 28  | 0.3790525   | —        | -1.3437307     | —        | 1x  |
| 2   | 29  | 0.3790520   | —        | -1.3435885     | —        | 1x  |
| 2   | 30  | 0.3790518   | .000006  | -1.3435431     | .0001628 | 2x  |
| 2   | 31  | 0.3790518   | .000005  | -1.3435300     | .0001315 | 3x  |
| 2   | 32  | 0.3790513   | .000016  | -1.3432041     | .0010873 | 3x  |
| 2   | 33  | 0.3790515   | .000007  | -1.3433885     | .0004434 | 4   |
| 2   | 34  | 0.3790519   | .000003  | -1.3435503     | .0000824 | 5   |
| 2   | 35  | 0.3790521   | .000004  | -1.3436142     | .0001314 | 5   |
| 2   | 36  | 0.3790519   | .000006  | -1.3435607     | .0001972 | 6   |
| 2   | 37  | 0.3790520   | .000001  | -1.3435822     | .0000276 | 7   |
| 2   | 38  | 0.3790520   | .000001  | -1.3435845     | .0000264 | 6   |
| 2   | 39  | 0.3790521   | .000002  | -1.3436174     | .0000616 | 4   |
Table 5. Sequences of amplitude estimates. Refer equation (5.2)

| n  | $d_2$  | $d_1$  | $b_1$  | $a_2$  | $a_1$  |
|----|--------|--------|--------|--------|--------|
| 29 | 0.0639 | -0.1878| -0.1999| 0.5584 | 1.17700|
| 30 | 0.0666 | -0.1879| -0.2022| 0.5590 | 1.17699|
| 31 | 0.0715 | -0.1881| -0.1980| 0.5579 | 1.17700|
| 32 | 0.0738 | -0.1882| -0.1999| 0.5584 | 1.17700|
| 33 | 0.0781 | -0.1883| -0.1963| 0.5574 | 1.17701|
| 34 | 0.0800 | -0.1884| -0.1979| 0.5578 | 1.17700|
| 35 | 0.0838 | -0.1885| -0.1947| 0.5570 | 1.17701|
| 36 | 0.0855 | -0.1885| -0.1960| 0.5573 | 1.17701|
| 37 | 0.0890 | -0.1886| -0.1932| 0.5566 | 1.17701|
| 38 | 0.0904 | -0.1887| -0.1943| 0.5569 | 1.17701|
| 39 | 0.0936 | -0.1888| -0.1919| 0.5563 | 1.17702|

Table 6. Sequences of amplitude estimates, with the exponent associated with $d_2$ changed from $-\frac{5}{2}$ to $-2$. Refer equation (5.2)

| n  | $d_2$  | $d_1$  | $b_1$  | $a_2$  | $a_1$  |
|----|--------|--------|--------|--------|--------|
| 29 | 0.0246 | -0.1902| -0.2004| 0.5585 | 1.17699|
| 30 | 0.0252 | -0.1903| -0.2017| 0.5589 | 1.17699|
| 31 | 0.0266 | -0.1906| -0.1985| 0.5580 | 1.17700|
| 32 | 0.0270 | -0.1906| -0.1994| 0.5583 | 1.17700|
| 33 | 0.0281 | -0.1908| -0.1969| 0.5576 | 1.17700|
| 34 | 0.0283 | -0.1909| -0.1974| 0.5577 | 1.17700|
| 35 | 0.0292 | -0.1910| -0.1952| 0.5571 | 1.17701|
| 36 | 0.0293 | -0.1910| -0.1955| 0.5572 | 1.17701|
| 37 | 0.0301 | -0.1912| -0.1937| 0.5568 | 1.17701|
| 38 | 0.0301 | -0.1912| -0.1939| 0.5568 | 1.17701|
| 39 | 0.0308 | -0.1912| -0.1923| 0.5564 | 1.17702|
Figure captions

Figure 1. Schematic representation of projections of self-avoiding walks onto the $y$ axis.

Figure 2. The 5 types of irreducible component from which self-avoiding walks are constructed.

Figure 3. The cross-section line defining the set of lattice bonds which specify the partial generating functions.
