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Enumeration of self-avoiding trails on a square lattice using a transfer matrix technique

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Abstract. We describe a new algebraic technique, utilizing transfer matrices, for enumerating self-avoiding lattice trails on the square lattice. We have enumerated trails to 31 steps, and find increased evidence that trails are in the self-avoiding walk universality class. Assuming that trails behave like $A\lambda^n n^{11/32}$, we find $\lambda = 2.720\,62 \pm 0.000\,006$ and $A = 1.272 \pm 0.002$.

1. History

Over the years, the study of the trails problem has provided an interesting counterpoint to the corresponding SAW problem. While self-avoiding walks are connected open non-intersecting paths on a lattice, and hence no site or bond may be visited more than once, lattice trails are open paths on a lattice which may re-visit sites, but not bonds. Thus SAWs are a proper subset of trails. First seriously studied by Malakis [1], a number of exact and numerical results were obtained by Guttmann [2,3].

It has been shown by Hammersley [4] that SAWs have a connective constant: that is some value μ such that if there are c_n SAWs of length n, then $\log \mu = \lim_{n\to\infty} \log(c_n)/n$ exists and is finite and non-zero. Later, Hammersley and Welsh [15] proved that $c_n = \mu^n \exp(O(\sqrt{n}))$.

These results were carried over to trails by Guttmann [2]. If t_n is the number of trails of length n, and λ denotes the connective constant for trails then $c_n \leqslant t_n$ and $\mu \leqslant \lambda$. It was also shown [2] that the critical behaviour is in the SAW universality class for trails on the honeycomb lattice, though no such proof has been found for the square lattice case. The earlier series were found to be rather poorly converged compared to SAW series of similar length, with the exponent of the trails generating function being $\gamma \approx 1.40$, compared to the SAW result $\gamma = \frac{43}{32} = 1.343\,75$. The connective constant was estimated as $\lambda = 2.7215 \pm 0.002$. This poor convergence prompted Guttmann and Osborn [5] to carry out a Monte Carlo study, using the Berretti–Sokal [6] algorithm, using walks up to 200 steps. They found $\gamma = 2.7205 \pm 0.0016$ and $\gamma = 1.348 \pm 0.11$. A biased

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estimate of the connective constant, assuming $\gamma = 1.343\,75$, gave the critical point estimate $\lambda = 2.720\,59 \pm 0.0008$. Recently Lim and Meirovitch [7] used an entirely different Monte Carlo algorithm, the scanning simulation method. They obtained the estimates $\lambda = 2.720\,58 \pm 0.000\,20$ and $\gamma = 1.350 \pm 0.012$.

In this work we report a substantial extension of the series expansion of the generating function for square lattice trails. The finite-lattice method plus transfer matrices described here allows 31 terms to be obtained on a work station (an IBM 6000/530 with 256MB of memory). The method is described below. The complexity of our algorithm is in fact worse than exponential, compared to λ^n required by a conventional enumeration algorithm, where n is the maximum number of steps. However for intermediate values of length, say 50–100 steps, it is in fact substantially faster. The detailed performance is discussed in section 2.7.

2. Algorithm

The algorithm for enumerating self-avoiding trails is very similar to the algorithm for enumerating self-avoiding walks described in [8]. We will summarize this process, expanding and pointing out the differences between walks and trails where appropriate. Where there is no difference, the word *paths* is used to denote either walks or trails.

2.1. Introduction

The basis of this method is the transfer matrix technique on a finite lattice. This enables one to count the total number of paths on a square lattice (or other type of lattice, with the appropriate modifications). We shall firstly discuss paths that can fit into a finite lattice.

The fundamental problem with enumerating self-avoiding paths is that the self-avoiding constraint is non-local. One cannot just say, for instance 'There are x number of ways of getting from $(0,0)$ to (a,b) and y number of ways to get from (a,b) to (c,d), so there must then be xy ways to get from $(0,0)$ to (c,d).' However, if we *could* do something like this, it could save a great deal of time, since xy is typically much larger than $x + y$—that is, it is faster to count x steps followed by y steps than it is to count xy steps.

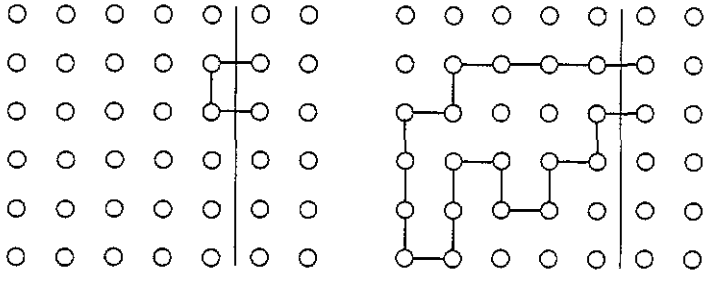


Figure 1. Two examples of a partial path, each with a boundary (vertical line) and the same boundary conditions.

If one draws a boundary line through the (finite) lattice, one notices that the self-avoiding constraint works independently on both sides. This means that it would be possible to work out, for all the possible boundary conditions, how many patterns to the left and right of the boundary there are that give those boundary conditions. A boundary condition is the set of bonds cut by the boundary line, plus a description of their interconnectedness. Thus, one can consider the two partial paths given in figure 1 as behaving in exactly the same manner, if all further growth takes place on the right of the boundary. The number of partial paths to the left and right with a given boundary can then be multiplied and summed over all boundaries to give the required number of paths.

Note that we usually do not want the total number of paths on a certain sized lattice, but rather the number of paths of a certain length on that lattice.

To cope with this, instead of just counting the number of partial paths to either side of the boundary, one can count the number of partial paths of n steps, g_n, and then make a generating function $G(x) = \sum_{n=0}^{\infty} g_n x^n$. Then, when one multiplies the generating functions for either side of the boundary, one ends up with a total generating function, from which the number of paths of the appropriate length can be easily extracted.

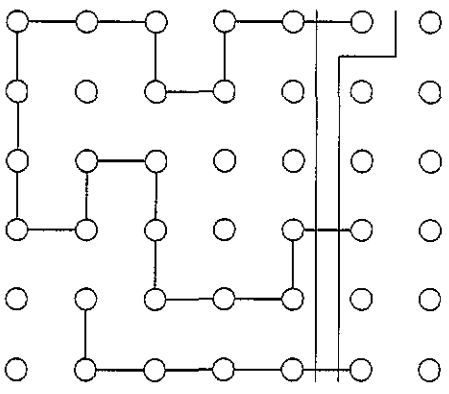


Figure 2. Two boundaries differing by only one site.

However, this leaves the tasks of actually counting those paths, and of matching them up. This task can be simplified by noticing that we could add in a second boundary (figure 2) separating just a single site.

Now, we have three independent areas. The matching process is however not much more complicated. First, one works out the generating functions for all possible boundary conditions on the left. Secondly, for each of the boundary conditions on the left, one works out which new paths can be created by adding this new point. This will create zero or more possible new paths to the left of the second line, with perhaps different generating functions. When two or more different 'first boundary' conditions create the same 'second boundary' condition, the generating functions should be added. An example of the new boundary conditions created is shown in figure 3.

This process can be represented as matrix multiplication. We start off with a column vector of generating functions, where each element corresponds to a particular (first) boundary condition. We then perform a linear transformation of this column vector to another column vector containing a generating function for each (second)

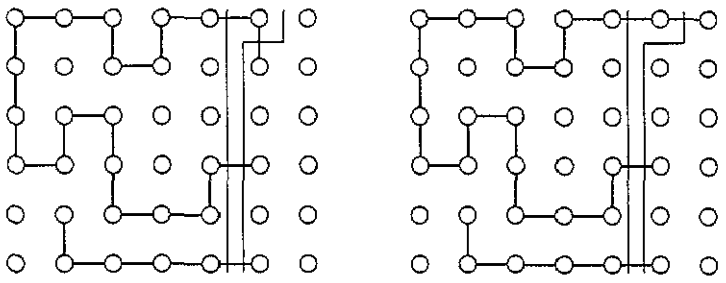


Figure 3. The two new partial paths resulting from moving the active boundary across one site. A third possibility is not to add any bonds and have two floating partial paths instead of one floating partial path and two connected path ends.

boundary condition. This is the same as multiplying on the left by a rectangular matrix. This is the reason for the name 'transfer matrix technique'. Note that the column matrices are very long, so this rectangular matrix will be exceedingly large. However, *there is no need to store this matrix as the matrix is very sparse, and* elements can be calculated on demand.

This process can add one extra point. But there is no reason that this process can not be continued to add a second point...or a third...or the rest of the lattice, one site at a time. Once the end of the lattice is reached, the boundary conditions are very simple to match: nothing is allowed to cross the end of the lattice. Similarly, there is no reason why one cannot start at the very beginning of the lattice. One then begins with only one initial boundary condition—no connections, and the trivial generating function 1. Thus one can generate all the possible paths using only the transfer matrix techniques. This means one never has to explicitly count paths. This process is potentially significantly faster than counting paths individually.

2.2. *Defining boundary conditions*

The boundary specification is called a 'signature' and is based on a series of numbers, one for each of the bonds crossed by the boundary line. For a lattice of width W bonds, there will be $W + 1$ (vertical line) or $W + 2$ (vertical line with a kink) of these bonds.

Each bond crossed may be characterized by one of three possibilities. Firstly, it may be unoccupied, in which case it is easy to specify. Assign it the number '0'. Secondly, the bond may be occupied, and lead to a dangling end. That is, the pathlet connected to the bond ends somewhere to the left of the boundary. This is also easy to specify—assign it the number '1'. Note that these assignments are arbitrary, there is no inherent meaning in this code. The third possibility is that the bond is occupied, and is connected (via some route to the left of the boundary) to some other bond on the boundary. In order to fully specify this, one must somehow uniquely define which bond it is connected to.

The arrangement of possible interconnections is severely limited in the self-avoiding walk case, as the pathlets cannot cross. This enables a very efficient encoding: if one labels the 'top' of a pathlet with a '2' and the bottom with a '3', then this will uniquely specify the way the bonds are connected. For, if there is a '2' at some point in the signature, one can find the corresponding '3' by moving down the signature until the next '3' is found, subject to the condition that every time a '2' is crossed,

one must ignore an extra '3'. So for instance, in the signature '232233', the first '2' matches the first '3', whilst the second '2' matches the last '3'. A computer can then store each code number for each bond as two binary bits, so for $W \leqslant 14$ the whole signature fits nicely into a 32 bit binary word, which is very convenient for current computers.

For self-avoiding trails, we do not have this nice restriction. Self-avoiding trails can cross themselves at a site, as it is only the bonds that have to avoid one another. This means that one cannot get away with a clever encoding of just two symbols. Indeed, no finite number of symbols will do for all values of W, as will be presently shown. This leaves the explicit option, where the code number for each bond specifies the index of the bond to which it is attached (plus 1). The index of a bond is the bond's position on the boundary—1 up to $W+2$ inclusive. The addition of one is to prevent mistaking a dangling end with a connection to the first bond. This means each bond will have a number from 0 to $W+3$ associated with it. If we restrict $W \leqslant 12$ in a computer program, then each bond fits into 4 bits, and the total signature is 56 bits, which is a little more clumsy to deal with, but not difficult.

Note that the specific numbers mentioned above for restrictions on W are in no way restrictions on the algorithm, just on a particular programming implementation. We only used $W = 7$ anyway, due to finite computer resources.

Paradoxically, the 'implicit' coding of the self-avoiding walk boundaries is significantly easier for a computer program to deal with than the 'explicit' encoding for the self-avoiding trails. This is due to the fact that most operations deal with local changes, when adding a site. These local changes are easy to implement with the implicit coding.

Note that in [8] we used a permutation of the numbering system described above for SAWS: we used '3' as the dangling end marker, and '1' and '2' for the loop ends. We have changed notation here for consistency.

The coding of the signatures is actually of vital importance, as the total time and memory requirements of the algorithm are polynomials in W times the number of different signatures (W^2 for space, and W^4 for time), as discussed in section 2.7.

For self-avoiding walks, an upper bound on the number of different signatures is obvious: 4^{W+2}, as there are 4 different possibilities for each bond, and $W+2$ possible bonds. Actually, there are significantly fewer than this since not all combinations are possible: one cannot have more than two floating ends (as it would be impossible to make them into a connected walk), and one cannot end a loop with a 3 before starting it with a 2. It turns out that the number of possible signatures grows like a polynomial in W times 3^W.

For self-avoiding trails, the situation is again worse. The number of possible boundary conditions can be evaluated exactly in a straight-forward manner. Let B_n be the number of boundary conditions for a strip of width n, and L_n the number of boundary conditions *excluding 'dangling' paths*. That is, all of the $n+2$ bonds on a boundary condition counted in L_n must either be unused bonds, or may be connected to another bond on the boundary. In [8] these were marked by a '3'. A formula for B_n in terms of L_n is easy to obtain: any boundary counted in B_n may have no dangling ends (giving a term L_n), or it may have one dangling end in any of $n+2$ places (giving a term of $(n+2)L_{n-1}$), or it may have two dangling ends giving a term of $(n+2)(n+1)L_{n-2}$. Thus we have

$$B_n = L_n + (n+2)L_{n-1} + (n+2)(n+1)L_{n-2}. \tag{2.1}$$

Now to work on an equation for L_n: the first bond may be unoccupied, giving a term of L_{n-1}, or it may be connected to one of $n+1$ other bonds, giving a term of $(n+1)L_{n-2}$, thus

$$L_n = L_{n-1} + (n+1)L_{n-2}. \tag{2.2}$$

Initial conditions are $L_{-1} = 1$, $L_{-2} = 1$ and $L_{-3} = 0$.

These are worrying equations as they grow faster than exponentially due to the $(n+1)L_{n-2}$ term in equation (2.2). This faster than exponential growth is the reason why no finite set of symbols could cope with encoding the connections for all values of W.

Actual values are given in table 1, along with the number s_n (taken from [8]) of possible boundary conditions for self-avoiding walks.

Table 1. Number of boundary conditions for trails (B_n) and for SAWS (s_n). Values for s_n come from [8].

n	L_n	B_n	s_n
−1	1	2	2
0	2	5	5
1	4	13	13
2	10	38	37
3	26	116	106
4	76	382	312
5	232	1 310	925
6	764	4 748	2 767
7	2 620	17 848	8 314
8	9 496	70 076	25 073
9	35 696	284 252	75 791
10	140 152	1 195 240	229 495

2.3. Irreducible components

Using the transfer matrix method directly is not as much of a saving as could be expected, due to the very large number of vectors. If we want to count all paths up to a maximum length of $2n+1$, then at first it looks as though a square $2n+1$ wide is needed to cope with a perfectly vertical path. However, it is possible to use the symmetry relation between the horizontal and vertical axes, so that only paths up to a width of n need to be calculated: for paths of width $n+1$ or greater, we can say that they must have height n or less, and thus their mirror images will have already been counted. More formally, if G_{ij} is the number of paths with i horizontal and j vertical steps, then $G_{ij} = G_{ji}$ and thus if we know G_{ij} for $i \leqslant 2n+1$ and $j \leqslant n$, we really know G_{ij} for all $i + j \leqslant 2n+1$. That is, we know the total number of paths of length up to $2n+1$ steps. This means that we could work with strips of width n, length $2n+1$ and obtain coefficients up to and including $2n+1$.

There is still a further improvement. Suppose that we break up all the paths (of vertical steps $\leqslant n = 2M+1$) into two classes, irreducible and reducible.

Irreducible paths have no place where a horizontal line could be drawn across the lattice intersecting exactly one vertical bond. As there are a maximum of $2M+1$ vertical bonds in the path, and there must be at least two vertical bonds for each unit

of width (to satisfy the irreducibility definition), these paths must all fit into a strip of width M bonds.

Reducible paths have at least one place where the horizontal line can be drawn, intersecting just one bond of the path. These paths have the nice property that the self-avoiding constraint will act independently both above and below this line. All that is needed is to calculate the number of self-avoiding paths above and below independently. This is a smaller problem, and indeed, can be further split up, until the entire path can be considered to be made up of an irreducible 'top' section, then one or more sections composed of a vertical bond and an irreducible 'middle' section, then finally a vertical bond and an irreducible 'bottom' section. As all of these irreducible subsections will have fewer than n steps, they will fit into a strip of width M.

All in all, these two optimizations allow calculations on a strip of width M bonds to provide the number of paths with widths up to $n = 2M + 1$ and thus paths with total number of bonds up to $2n+1 = 4M+3$. Since the number of partial generating functions rises exponentially with strip width, these two optimizations reduce the complexity of the problem enormously.

However, it makes the counting task a little more difficult: we have to extract these 'top', 'middle' and 'bottom' sections individually. To facilitate this, the irreducible paths can be named as described in table 2, based upon their starting and end points. Note that a distinction is made here between paths and routes. A *path* has a specific starting point: a *route* does not. This means that there are exactly half as many routes as paths.

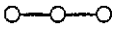
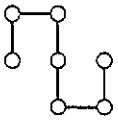
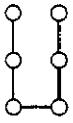
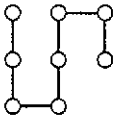
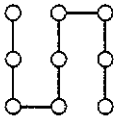
Note that routes with two bottom ends are not included, as they are the same (in number and shape) as R, and similarly routes with one bottom end and one middle end are not given a name as they are covered by S. Note that all the routes above are irreducible.

The name in this table is the name of the generating functions associated with that variable in this paper. There are six generating functions associated with each letter in this paper, as per the following pattern:

- $Q(u,w)$ is the generating function for irreducible routes of the required shape with the power of u giving the number of horizontal bonds, and w representing vertical bonds.
- $Q_W(u,w)$ is the same, except only for those irreducible routes of width exactly W.
- $Q^*(u,w)$ is the generating function for *all* (i.e. both reducible and irreducible) routes of the required shape.
- $Q^*_W(u,w)$ is the same, except for all routes with width exactly W.
- $Q(u,w,z)$ is the generating function for irreducible routes of the required shape with the power of u giving the number of horizontal bonds, w representing vertical bonds, and z the total width.
- $Q^*(u,w,z)$ is the generating function for all routes of the required shape with the power of u giving the number of horizontal bonds, w representing vertical bonds, and z the total width.

Note that the same terminology applies to variables other than Q, with *routes* changed to paths where appropriate. The three variable generating function is the most general: the width W generating functions can be extracted from the appropriate power of z, and the generating functions in two variables can be produced

Table 2. Irreducible paths described by their starting and end points.

Description	Picture	Name	Lowest power in w for width M
Path with no vertical bonds		P	N/A
Route with two middle ends		Q	w^{2M}
Route with two top ends		R	w^{2M}
Route with one top, one middle end		S	w^{2M+1}
Route with one top, one bottom end		T	w^{3M}

from the functions in three variables by setting $z = 1$. That is

$$Q(u,w) = Q(u,w,1) \qquad Q(u,w,z) = \sum_{n=0}^{\infty} z^n Q_n(u,w).$$

Note that if a path is on a strip the width of which is too small for the definition to make sense, then the corresponding generating function is zero: i.e. Q_0, Q_1, R_0, S_0, S_1, and T_0 are all zero.

Of these five functions, P is easy to determine. There is one horizontal path of length zero, and two paths of every other length (one in each direction). Thus

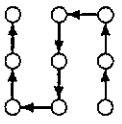
$$P(u,w,z) = 1 + 2u + 2u^2 + 2u^3 + \cdots = \frac{1+u}{1-u}.$$

Now define another variable, X. This will represent the total number of irreducible middle sections. That is, the number of ways of going from a point at the bottom of an irreducible section to a point on the top. Note that every element of T can be considered as a path *restricted so as to not go below the starting point*. Thus, T copes with all the parts of X of width at least one. For the zero width case, we just want paths from one point on a line to another point P, thus

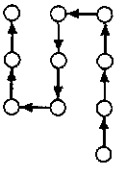
$$X = T + P.$$

This is the reason for defining P to be paths, whilst Q, R, S, and T are routes.

This is a typical X



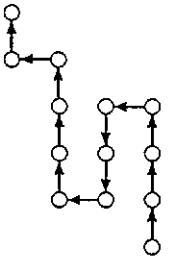
and this is the corresponding wzX



X refers to just a single irreducible middle section. This can be extended to an arbitrary middle section by noting that a 'middle section' can be formed from either a vertical bond (wz), or two vertical bonds with an X in between, ($wzXwx$), or any number of extra wzX terms. Define a new variable V to be a total (reducible) 'middle section', then

$$V = wz\,(1 + wzX + (wzX)^2 + (wzX)^3 + \cdots) = \frac{wz}{1 - wzX}. \quad (2.3)$$

A V can be considered to be a generalization of a vertical bond: it is a reducible path without either the top or bottom irreducible components. A typical element of V is shown below. The arrows indicate that the V is intended to be used as *part* of a path, not as something in its own right.



Note that the top and bottom of a V are *always* vertical bonds, so a V can attach to *any* irreducible component which has an end at its top or bottom. This can be a P, an R, an S or a T. Note that the R has two ends to which connections can be made, so we must count it twice. P is not counted twice since it is a path, not a route. Define the generating function of end components, E as

$$E = P + 2R + S + T.$$

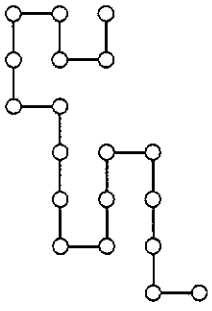
Now all the reducible routes can be calculated. Each consists of one end piece, E, a joint V and another end piece E. Thus reducible routes are EVE. Irreducible routes (with some vertical component, i.e. not P) are $Q + 2R + 2S + T$. R and S are counted twice to allow for routes with two bottom ends or one bottom and one

middle end respectively. To get the total number of paths then, we take the number of paths with no vertical component, P, and add in twice the number of routes with vertical components. This gives

$$C = P + 2(Q + 2R + 2S + T + EVE)$$

as the total number of paths.

This is a typical reducible path, made up from a TVP



where the V in this case is $wzPwzTwz$.

2.4. Obtaining the irreducible components

So far only $P(u, w, z)$ is known. In order to calculate the number of self-avoiding paths up to length $4M+3$, $Q(u, w)$, $R(u, w)$, $S(u, w)$ and $T(u, w)$ must be known accurate to u^{4M+3} and to w^{2M+1}.

Suppose that it were possible to obtain the starred polynomials Q^*, R^*, S^* and T^* as functions of three variables. Then $R = R^*$, as all paths starting from the top and ending at the top are irreducible.

Calculating the others is a little more difficult. Consider the generalization of X to X^*. X^* will be equal to the sum of the irreducible parts X, plus reducible paths starting at the bottom and ending at the top. These are expressible as XVX, so we have $X^* = X + XVX$. Using equation (2.3), this can be inverted to give

$$X = \frac{X^*}{1 + wzX^*} \tag{2.4}$$

which can be expanded in a formal binomial series to give

$$X = X^* \left(1 - wzX^* + w^2z^2X^{*2} - \cdots\right).$$

If X^* is known to some order in u and w for powers up to z^M, then X can be determined to the same order. Since X is made up of P (which is zero for widths other than 0), and T, which has the lowest power of w being three times the power of z, order is preserved up to w^{3M+2} and to the original order in u. Thus, if X^* is known to u^{4M+3} and v^{2M+1}, this is preserved in the calculation of X. So, by using the third variable, one can go from X^* to X, and thence T. Without using the third variable z, the generating function X^* would only be correct to terms of order w^M rather than w^{2M+1}.

Similarly, if we define $Y = 2R + S$ (connections at the bottom, but not the top), then $Y^* = 2R^* + S^* = 2R + S + XVY = Y(1 + XV)$, so there is an expression for Y similar to equation (2.4)

$$Y = \frac{Y^*}{1 + XV}.$$

One can then obtain Y and thence S from Y^* and hence S^*, in a manner similar to that used to obtain T from T^* via X and X^*.

Lastly, $Q^* = Q + YVY$ so

$$Q = Q^* - YVY$$

and Q can also be obtained in a similar manner.

This means that all the irreducible components can be obtained from reducible components given the full three variable information, and accuracy to

- M in z (i.e. to width M)
- $2M + 1$ in w
- $4M + 3$ in u.

2.5. Obtaining reducible components

Suppose that we could count all the paths on a certain finite lattice with constraints upon where the paths can start or end. Define the generating function in variables u to order $4M + 3$ and w to order $2M + 1$ for paths on a strip of width K as $G_K(a, b, c)$, where a, b, and c are $+$ or $-$ depending upon whether one can start or end paths on the top of the strip, the bottom of the strip, and/or the middle of the strip respectively. Ensure that all paths included in these generating functions start flush at the left of the lattice so that we do not need to worry about uniqueness in the horizontal direction.

Now, by considering how the walks that fit into the strip can be made up of the reducible functions defined above, the latter can be defined as an invertible linear combination of the former. One inverts this relation and gets the reducible components needed in section 2.4 from the $G_K(+,-,-)$, $G_K(+,+,-)$, $G_K(-,-,+)$ and $G_K(+,-,+)$, for K from 0 to M.

These relations are (as taken from [8])

$$R_m = G_m(+,-,-) - G_{m-1}(+,-,-)$$

$$Q^*_m = G_m(-,-,+) - G_{m-1}(+,-,+) - \sum_{n=1}^{m-1} (Q^*_n + R_n + S^*_n)$$

$$S^*_m = G_m(+,-,+) - G_{m-1}(+,-,+) - G_m(+,-,-) - G_{m-1}(+,-,-) - \tfrac{1}{2}(P-1) - Q^*_m - \sum_{n=1}^{m-1} (Q^*_n + 2 * S^*_n + T^*_m)$$

$$T^*_m = G_m(+,+,-) - 2G_m(+,-,-).$$

2.6. Counting paths on strips

The transfer matrix technique can be used to obtain the generating functions G_K that are needed in section 2.5.

Suppose we are working on a lattice of width W and length $4W+3$. As mentioned before, one starts with one partial generating function (boundary to the left of the entire lattice, no bonds used, generating function 1). Then add on sites as described in the next paragraph one at a time, working along the matrix column by column. At each site one stores for each valid signature the partial generating function. After processing the first column, one can remove the signature with no bonds occupied, as any animal based upon this signature will not lie flush against the left of the lattice, and by removing it we satisfy the horizontal uniqueness criterion.

To process a site, one cycles through all the stored signatures, processing each individually, creating a new set of signatures. Note that two or more signatures may produce the same signature after processing. In this case the partial generating functions for these two signatures should be added.

All that is left is to describe exactly what to do when each site is added for a particular signature. The site that is being added will have two bonds coming in (to the left of the new boundary), and another two bonds leaving (to the right).

One must firstly see if the walk can be finished at this point, and if so, add in the partial generating function to a total generating function which will give the final G_K once all sites have been processed. In order to be able to accumulate a partial walk, two conditions must be satisfied. Firstly, there must be no occupied bonds in the signature other than those coming into the bond being processed. Secondly, one of the three following conditions must hold

- There must be a single dangling end coming in to the site being processed (type '1' in the signature coding), and it is valid to start or stop a path at this point (determined by the + or − parameters in the particular G_K being computed.
- Or there may be two dangling ends that connect at this site.
- Or (only in the case of trails) there may be a loop completed at this site and it is valid to start or stop a path at this point.

We will first discuss the possibilities for the new signatures if one cannot start or stop a path at the site being processed.

If one is counting walks, and there is only one bond going into the site, then that one bond must emerge from either of the two bonds coming out of the site. This gives two new signatures, one with the old generating function multiplied by w (emerging vertically), and one with the old generating function multiplied by u (emerging horizontally). In future we will not mention these multiplications.

Again for walks, one may have both bonds entering the site occupied. In this case neither output bond may be occupied, as one cannot have more than two occupied bonds touching a site for self-avoiding walks. What happens depends upon the specific case. If the two bonds are attached together, then a loop has been formed which is illegal, so no signatures are generated. If the two bonds are dangling ends, then attaching them would make an entire dangling path, which is not allowed. In the remaining cases, one does produce a new valid signature, and one must adjust the coding for the bond(s) in the signature to which the just processed bonds were attached.

Again for walks, if there are no bonds coming in, then there are two possibilities:

no bonds coming out, or a new path being started at this point—that is two bonds coming out and connected to each other.

Further possibilities exist if one can stop or start from the site being processed.

For walks with no bonds coming in, one can now have one dangling end coming out of either of the two outgoing bonds. With one bond coming in which is not a dangling bond, the pathlet it belongs to can be terminated at this site, and the bond to which it is attached elsewhere in the signature becomes a dangling bond. Note that each of these steps increases the number of dangling bonds in the signature, and one must check that the total number of dangling bonds does not exceed two, as this would mean that any path one tries to construct must have at least three ends!

These are summarized in table 2 of [8].

For trails, the situation is significantly more complicated, as bond loops and crossings are allowed, but the basic idea remains the same.

First, consider what can be done without starting or stopping.

The same possibilities as in the walks case (without stopping or starting at the site being processed) hold, with some extra possibilities when there are two bonds coming in. Firstly, both bonds could 'bounce' and come out as two bonds with the same connections. Secondly, they could cross, and come out as two bonds with interchanged connections. Thirdly, if the two bonds coming in meet, and in the walks case would have produced no bonds coming out, one may also have two new connected bonds coming out, as occurred in the walks case when no bonds went in.

If one is allowed to start or stop at the site being processed, things get much more complicated. The actions can best be described by two stages.

In the first stage, associated with terminating incoming pathlets, one forms all the possibilities already described, and adds in the following possibilities:

- For one bond entering which is not an dangling end, the pathlet may be terminated at this site, and the other end of the pathlet converted to a dangling end (as was done for walks). No occupied bonds emerge.
- For two bonds entering, one a dangling end, and the other a pathlet, the pathlet may terminate (making the other end of the pathlet a dangling bond) and the dangling end can continue from either of the two new bonds.
- For two ends of the same pathlet entering, one end may terminate at the current site, and the other end (now a dangling end) may take either of the two new bonds. As either end of the pathlet may terminate, there are four new signatures produced.
- For two ends of different pathlets entering, there are the same four possibilities as above, except that this time it is a pathlet leaving, not a dangling end, and some other bond in the signature will become a dangling end. A fifth possibility is for both incoming pathlets to terminate, producing two dangling ends elsewhere in the signature and no bonds coming out.

In the first and last case above, there is the possibility of no bonds coming out. Again, one can add a new two bond loop in both cases as in the walks case when no bonds went in.

The second stage is associated with adding dangling ends at the leaving stage. If any of the signatures formed from the first stage have either or both of the outgoing bonds unoccupied, either or both may be filled with dangling ends.

Of course, when forming new dangling ends, one must remember the constraint that the total number of dangling ends in the signature may not exceed two.

2.7. Algorithm complexity

One now has all the ingredients for the algorithm. One uses the transfer matrix technique to get all the G_K terms for K going up to some value W (section 2.6), then obtain the reducible generating functions (section 2.5) and thus obtain the irreducible generating functions and final answer (section 2.4).

Of these three stages, the first (section 2.6) is exceedingly time and memory consuming, whilst the second (section 2.4–5) is fast (polynomial in W time) and uses little memory.

Since the first stage is the bottleneck, we shall discuss it exclusively in terms of complexity.

The total memory required will be bounded by the number of possible boundary conditions, multiplied by the total space per generating function (proportional to W^2), multiplied by two, since one may need to store both the incoming and outgoing partial generating function. In practice, this last factor is nowhere near as high as two, since as soon as a signature has been fully processed, the data associated with it may be discarded.

The total time required is proportional to the total amount of memory that needs to be processed (as above) times the number of sites that have to be processed (proportional to W^2), times the average number of new signatures per old signature. This last factor is pretty much independent of W. For trails it is significantly larger than walks.

The basic result is that the time and memory requirements are a small polynomial times the number of boundary conditions. The number of boundary conditions is therefore the most significant factor in the complexity of this algorithm.

For self-avoiding walks, the number of boundary conditions grows like a polynomial in W times 3^W. Thus the dominant complexity of this method for self-avoiding walks is $3^{n/4}$, where n is the number of steps required. This comes from the fact that $n = 4W + 3$. The alternative, direct enumeration, grows like λ^n, where λ is the connective constant for self-avoiding walks. Note that λ is significantly greater than $3^{1/4}$ (approximately twice $3^{1/4}$ in fact), so this algorithm is exponentially faster than direct enumeration.

For trails, the situation is not as good. The analysis in section 2.2 shows that the number of boundary conditions grows faster than exponentially. Thus, for very long trails, direct enumeration will be a more efficient algorithm! However, consulting table 1 shows that trails are not all that much worse than walks for small values of W. So for small values of W, this transfer matrix method is actually more efficient than direct enumeration. Fortunately, the values of W for which this algorithm is faster than directed enumeration are such that this algorithm is faster for n at least 50, which is far beyond the capacity of current computers.

This algorithm is also amenable to parallelization in the same manner as the self-avoiding walk algorithm described in [8].

This algorithm was implemented in a C program using modular arithmetic, and was used to obtain trails of up to 31 steps. They are given in table 3.

3. Analysis of series

The method of analysis used is based on first- and second-order differential approximants. It was used in previous papers [8, 9, 10] in which the related SAW

Table 3. Numbers of trails t_n of n steps.

n	t_n	n	t_n	n	t_n
0	1	10	60 092	21	4 742 946 484
1	4	11	169 092	22	13 123 882 524
2	12	12	474 924	23	36 274 940 740
3	36	13	1 329 188	24	100 226 653 420
4	108	14	3 715 244	25	276 669 062 116
5	316	15	10 359 636	26	763 482 430 316
6	916	16	28 856 252	27	2 105 208 491 748
7	2 628	17	80 220 244	28	5 803 285 527 724
8	7 500	18	222 847 804	29	15 986 580 203 460
9	21 268	19	618 083 972	30	44 028 855 864 492
		20	1 713 283 628	31	121 187 822 490 084

problem was studied, and is described in detail in [11]. In summary, we construct near-diagonal inhomogeneous differential approximants, with the degree of the inhomogeneous polynomial increasing from one to eight in steps of one. For first-order approximants ($K = 1$), twelve approximants are constructed that utilize 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 ($K = 2$), eight distinct approximants are constructed for each value of N. We find that as the number of series terms increases, the estimate of the critical exponent decreases. We show below that this is due to rather strong correction-to-scaling terms, much stronger than for the SAW case. Because of this, the estimates we quote below should be treated as over-estimates of the exponent and critical point

$$x_c = 0.367\,597 \pm 0.000\,02 \qquad \gamma = 1.352 \pm 0.01 \qquad (K = 1)$$

$$x_c = 0.3676 \pm 0.0001 \qquad \gamma = 1.348 \pm 0.008 \qquad (K = 2).$$

These results provide some support for the view that the trails are in the SAW universality class. The critical point estimate can be refined if we assume that $\gamma = 1.343\,75$ exactly, which is the SAW value. 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

$$x_c = 0.367\,564 \pm 0.000\,008 \qquad (K = 1)$$

$$x_c = 0.367\,562 \pm 0.000\,007 \qquad (K = 2).$$

These are combined to give our best estimate for the connective constant $\lambda = 1/x_c = 2.720\,62 \pm 0.000\,06$, which is in agreement with previous estimates, but rather more accurate than any previous estimate.

The much slower rate of convergence of the trails series critical point estimates compared to the corresponding SAW estimates is presumably due to stronger 'correction-to-scaling' terms. We have investigated this possibility using three different methods. Firstly, we used the method of Baker and Hunter [12] which transforms the series so that poles of the Padé approximants to the transformed series furnish estimates of the reciprocals of the exponents. However we found that the singularity on the negative real axis at $-x_c$ masked the presence of any confluent singularity at x_c. Accordingly, we split the series in two, treating the odd and even subsequences as independent series. In this way, we found exponents with the values ≈ 1.35 and ≈ 1.0 from the even sub-sequence. The smaller exponent was not well identified however. This implies a correction-to-scaling exponent of ≈ 0.35. The odd subsequence gave no evidence of any exponent apart from the leading one.

The next method we used was the method of Adler *et al* [13], in which a correction-to-scaling exponent is assumed, and then a transformation is applied which maps this non-analytic correction term to an analytic correction term. Padé analysis of the transformed series should then give the correct leading exponent. We tried various values of the correction-to-scaling exponent, and found that a value around 0.75 resulted in a series which gave the correct critical exponent of $\gamma = 1.343\,75$.

The third method is the same as that used in our recent study of SAWs [8]. In that method we *assume* the correction-to-scaling exponent, and fit the series coefficients to the assumed form. The fit is judged reasonable if the sequences of amplitude estimates appear to converge well. This is not a particularly sensitive method, but is useful in that it does provide amplitude estimates as well. From the two values of the correction-to-scaling exponent found above, we tried an intermediate value of 0.5. Given that the SAW exponent appears to be 1.5, this seemed a reasonable thing to try. As well as the correction-to-scaling term, there is another singularity on the negative real axis. For SAWs, Guttmann and Whittington [14] showed that this was at $x = -x_c$. That proof applies *mutatis mutandis* to trails. We assume that universality of exponents applies to non-physical singularities also—a result supported by our series analysis. Then the singularity on the negative real axis will also have the same exponent as the energy at the physical singularity—as for SAWs—and so we expect the generating function for trails to behave like

$$T(x) = \Sigma t_n x^n \sim A(x)(1-\lambda x)^{-43/32}[1+B(x)(1-\lambda x)^{\Delta}+\cdots]+D(x)(1+\lambda x)^{+1/2}.$$

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

$$t_n \sim \lambda^n[a_1 n^{11/32} + b_1 n^{11/32-\Delta} + (-1)^n d_1 n^{-3/2}]. \tag{3.1}$$

The three amplitudes, a_1, b_1, d_1 come from the leading singularity, the correction-to-scaling term and the term on the negative real axis respectively. A small program written in Mathematica was used to fit successive triples of coefficients, c_{n-2}, c_{n-1} and c_n for $n = 6, 7, 8, \ldots, 31$. The results (with $\Delta = \frac{1}{2}$) are shown in table 4.

At first sight, these appear to be converging rather well. Closer inspection reveals that the sequences have a turning point at around $n = 29$. We next tried a higher value of Δ, choosing $\Delta = 0.75$ in agreement with the prediction of the transformation method of Adler *et al* cited above. The results are shown in table 5.

Table 4. Sequences of amplitude estimates assuming $\Delta = \frac{1}{2}$. Refer to equation (3.1).

n	d_1	b_1	a_1
21	0.0289	−0.1805	1.2795
22	0.0309	−0.1833	1.2801
23	0.0296	−0.1849	1.2805
24	0.0311	−0.1868	1.2809
25	0.0306	−0.1874	1.2810
26	0.0313	−0.1885	1.2812
27	0.0310	−0.1889	1.2813
28	0.0314	−0.1894	1.2814
29	0.0315	−0.1893	1.2814
30	0.0316	−0.1894	1.2814
31	0.0319	−0.1890	1.2813

Table 5. Sequences of amplitude estimates assuming $\Delta = \frac{3}{4}$. Refer to equation (3.1).

n	d_1	b_1	a_1
21	0.0281	−0.2544	1.2661
22	0.0316	−0.2615	1.2668
23	0.0289	−0.2670	1.2673
24	0.0318	−0.2727	1.2679
25	0.0298	−0.2765	1.2683
26	0.0321	−0.2809	1.2687
27	0.0303	−0.2878	1.2690
28	0.0321	−0.2902	1.2692
29	0.0309	−0.2902	1.2695
30	0.0323	−0.2930	1.2697
31	0.0313	−0.2949	1.2698

These sequences of amplitudes appear to be converging reasonably well, and support the earlier finding that the correction-to-scaling exponent is around 0.75. If this is correct, we can extrapolate the above sequences and find $a_1 = 1.272 \pm 0.002$, $b_1 = -0.32 \pm 0.02$ and $d_1 = 0.035 \pm 0.004$. Even if the correction-to-scaling exponent were not as estimated, the leading amplitude is still likely to be within the quoted range.

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References

[1] Malakis A 1975 *J. Phys. A: Math. Gen.* **8** 1985
[2] Guttmann A J 1985 *J. Phys. A: Math. Gen.* **18** 567–73
[3] Guttmann A J 1985 *J. Phys. A: Math. Gen.* **18** 575–88
[4] Hammersley J 1957 *Proc. Camb. Phil. Soc.* **53** 642
[5] Guttmann A J and Osborn T R 1988 *J. Phys. A: Math. Gen.* **21** 513–17
[6] Berretti A and Sokal A D 1985 *J. Stat. Phys.* **40** 483

[7] Lim H A and Meirovitch H 1991 *Phys. Rev.* A **39** 4176–85
[8] Conway A R, Enting I G and Guttmann A J 1993 *J. Phys. A: Math. Gen.* **26** 1519–34
[9] Guttmann A J 1987 *J. Phys. A: Math. Gen.* **20** 1839–54
[10] Guttmann A J and Jian Wang 1991 *J. Phys. A: Math. Gen.* **24** 3107–9
[11] Guttmann A J 1989 *Phase Transitions and Critical Phenomina* vol 13, ed C Domb and J Lebowitz (New York: Academic)
[12] Hunter D L and Baker G A Jr 1979 *Phys. Rev.* B **19** 3808
[13] Adler J, Moshe M, and Privman V 1981 *J. Phys. A: Math. Gen.* **14** L363
[14] Guttmann A J and Whittington S G 1978 *J. Phys. A: Math. Gen.* **11** 721–9
[15] Hammersley J M and Welsh D J A 1962 *Q. J. Math.* Oxford Series 2 **13** 108