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Self-avoiding walks crossing a square

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Abstract

We study a restricted class of self-avoiding walks (SAWs) which start at the origin (0, 0), end at (L, L), and are entirely contained in the square $[0, L] \times [0, L]$ on the square lattice $\mathbb{Z}^2$. The number of distinct walks is known to grow as $\lambda^{L^2+o(L^2)}$. We estimate $\lambda = 1.744\,550 \pm 0.000\,005$ as well as obtaining strict upper and lower bounds, $1.628 < \lambda < 1.782$. We give exact results for the number of SAWs of length $2L + 2K$ for $K = 0, 1, 2$ and asymptotic results for $K = o(L^{1/3})$. We also consider the model in which a weight or *fugacity* x is associated with each step of the walk. This gives rise to a canonical model of a phase transition. For $x < 1/\mu$ the average length of a SAW grows as L, while for $x > 1/\mu$ it grows as L^2. Here μ is the growth constant of unconstrained SAWs in $\mathbb{Z}^2$. For $x = 1/\mu$ we provide numerical evidence, but no proof, that the average walk length grows as $L^{4/3}$. Another problem we study is that of SAWs, as described above, that pass through the central vertex of the square. We estimate the proportion of such walks as a fraction of the total, and find it to be just below 80% of the total number of SAWs. We also consider Hamiltonian walks under the same restriction. They are known to grow as $\tau^{L^2+o(L^2)}$ on the same $L \times L$ lattice. We give precise estimates for τ as well as upper and lower bounds, and prove that $\tau < \lambda$.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

We consider the problem of self-avoiding walks on the square lattice $\mathbb{Z}^2$. For walks on an infinite lattice, it is generally accepted [14] that the number of such walks of length n, equivalent up to a translation, denoted by c_n, grows as $c_n \sim \text{const}\,\mu^n n^{\gamma-1}$, with metric properties, such as the mean-square radius of gyration or mean-square end-to-end distance growing as $\langle R^2 \rangle_n \sim \text{const}\, n^{2\nu}$, where $\gamma = 43/32$ and $\nu = 3/4$. The growth constant μ is lattice dependent, and for the square lattice is not known exactly, but is indistinguishable numerically from the unique positive root of the equation $13x^4 - 7x^2 - 581 = 0$. We denote the generating function by $C(x) := \sum_n c_n x^n$. It will be useful to define a second generating function for those SAWs which start at the origin $(0, 0)$ and end at a given point (u, v), as $G_{(0,0;u,v)}(x)$. In terms of this generating function, the *mass* $m(x)$ is defined [14] to be the rate of decay of G along a coordinate axis,

$$m(x) := \lim_{n\to\infty} \frac{-\log G_{(0,0;n,0)}(x)}{n}. \tag{1}$$

Here, we are interested in a restricted class of square lattice SAWs which start at the origin $(0, 0)$, end at (L, L), and are entirely contained in the square $[0, L] \times [0, L]$. A *fugacity*, or weight, x is associated with each step of the walk. Historically, this problem seems to have led two largely independent lives. One as a problem in combinatorics (in which case the fugacity has been implicitly set to $x = 1$), and one in the statistical mechanics literature where the behaviour as a function of fugacity x has been of considerable interest, as there is a fugacity-dependent phase transition.

The problem seems to have first been seriously studied as a mathematical problem by Abbott and Hanson [1] in 1978, many of whose results and methods are still powerful today. A key question considered both then and now, is the number of distinct SAWs on the constrained lattice, and their growth as a function of the size of the lattice. Let $c_n(L)$ denote the number of n-step SAWs which start at the origin $(0, 0)$, end at (L, L) and are entirely contained in the square $[0, L] \times [0, L]$. Further, let $C_L(x) := \sum_n c_n(L)x^n$. Then $C_L(1)$ is the number of distinct walks from the origin to the diagonally opposite corner of an $L \times L$ lattice. In [1], and independently in [18], it was proved that $C_L(1)^{1/L^2} \to \lambda$. The value of λ is not known, though bounds and estimates have been given in [1, 18]. One of our purposes in this paper is to improve on both the bounds and the estimate.

Like so many problems in lattice statistics, this one owes a debt to J M Hammersley. A closely related problem to the one considered here is discussed in [15], which is in turn devoted to problems posed by Hammersley. However, the earliest mention of this problem appears to be by Knuth [12], who calculated the number of SAWs crossing a 10×10 square by Monte Carlo methods, and estimated the number to be $(1.6 \pm 0.3) \times 10^{24}$. It is now known, see table 2 below, that the correct answer is $1.5687\ldots \times 10^{24}$. A related problem was studied by Edwards in [7]. He considered a SAW starting at a point denoted the origin with the endpoint a distance L from the origin, and no other points at distance L or greater. Let $g(L)$ denote the number of such SAWs. Then Edwards proved that $\lim_{L\to\infty} g(L)^{(1/L^2)}$ exists and lies between 2.3 and 5.0. In our notation, Edwards has proved that $1.53 < \lambda < 2.24$. Edwards also proved that the same limit holds for a SAW from the origin to the boundary of any convex, bounded subset of $\mathbb{Z}^2$. His numerical work led him to suggest that λ is about 1.77. Our best estimate, given below, is 1.744 550(5).

The problem of Hamiltonian paths on an $L \times M$ rectangular grid, going from $(0, 0)$ to (L, M) has also been considered previously. Earlier work is described in [4], where Collins and Krompart also give generating functions for the number of such paths on grids with $M = 1, 2, 3, 4, 5$. In [10] Jacobsen and Kondev gave a field-theoretical estimate of the growth constant for Hamiltonian SAWs on the square lattice, which must fill a square, as $1.472\,801 \pm 0.000\,01$.

In the statistical mechanics literature, the problem appears to have been introduced by Whittington and Guttmann [18] in 1990, who were particularly interested in the phase transition that takes place as one varies the fugacity associated with the walk length. All walks on lattices up to 6×6 were enumerated, and the estimate $\lambda = 1.756 \pm 0.01$ was given. At a critical value, x_c the average walk length of a path on an $L \times L$ lattice changes from $\Theta(L)$ to $\Theta(L^2)$, where we define $\Theta(x)$ as follows. Let $a(x)$ and $b(x)$ be two functions of some variable x. We write that $a(x) = \Theta(b(x))$ as $x \to x_0$ if there exist two positive constants κ_1 and κ_2 such that, for x sufficiently close to x_0,

$$\kappa_1 b(x) \leqslant a(x) \leqslant \kappa_2 b(x).$$

In [18] the critical fugacity was proved to be at least $1/\mu$, its value was estimated numerically and was conjectured to be $x_c = 1/\mu$, and in [13] the conjecture was proved by Madras.

The problem was subsequently taken up by Burkhardt and Guim [2], who extended the enumerations given in [18] to 9×9 lattices, and used their data to give the improved estimate $\lambda = 1.743 \pm 0.005$. By considering SAW as the $N \to 0$ limit of the $\mathrm{O}(N)$ model of magnetism, Burkhardt and Guim show that the conjecture $x_c = 1/\mu$ made in [18] on numerical grounds follows directly, though this is not a proof, unlike the subsequent result of Madras [13].

They also gave a scaling *ansatz* for the behaviour of $C_L(x)$ for L large in the vicinity of $x = x_c$. They proposed

$$C_L(x) \sim L^{-\eta_c} f[L^{1/\nu}(x_c - x)] \tag{2}$$

where $\nu = 3/4$, as described above, and $\eta_c = 5/2$ is the corner exponent of the magnetization [3], given by Cardy's [3] result $\eta_c(\theta) = \frac{\pi}{\theta}\eta_\parallel$, for a wedge-angle θ, which is $\pi/2$ in this case. $\eta_\parallel = 5/4$ is the surface exponent that characterizes the decay of spin–spin correlations parallel to the boundary in the semi-infinite geometry, corresponding to wedge-angle π. Consequences of this scaling ansatz include the following predictions:

$$\begin{aligned} &C_L(x_c) \sim \text{const}\, L^{-\eta_c} \\ &\langle n(x_c, L)\rangle = x\frac{\partial}{\partial x}C_L(x_c) \sim \text{const}\, L^{1/\nu} \\ &\langle (n(x_c, L) - \langle n(x_c, L)\rangle)^2\rangle = \left(x\frac{\partial}{\partial x}\right)^2 \ln C_L(x_c) \sim \text{const}\, L^{2/\nu}. \end{aligned} \tag{3}$$

They tested these results from their numerical data, and found them well supported. We provide even firmer support for these results on the basis of radically extended numerical data. Equation (3) has also previously been given by Duplantier and Saleur [6].

Burkhardt and Guim also considered a generalization of the problem considered here by including a second fugacity, associated with steps in the boundary. This allows the problem of adsorbing boundaries to be studied. We will not discuss this aspect of the problem further, except to note that in [2] a full scaling theory is developed, and the predictions of the theory are tested against numerical data.

In [1] the slightly more general problem of SAW constrained to an $L \times M$ lattice was considered, where the analogous question was asked: How many non-self-intersecting paths are there from (0, 0) to (L, M)? If one denotes the number of such paths by $C_{L,M}$, it is clear that, for M finite, the paths can be generated by a finite-dimensional transfer matrix, and hence that the generating function is rational [17]. Indeed, in [1] it was proved that

$$G_2(z) = \sum_{L\geqslant 0} C_{L,2} z^L = \frac{1 - z^2}{1 - 4z + 3z^2 - 2z^3 - z^4}, \tag{4}$$

(where here we have corrected a typographical error). It follows that $C_{L,2} \sim \text{const}\, \lambda_2^{2L}$, where $\lambda_2 = \sqrt{\frac{2}{\sqrt{13}-3}} = 1.817\,35\ldots.$

In this paper, we also consider two further problems which can be seen as generalizations of the stated problem. Firstly, we consider the problem where SAWs are allowed to start

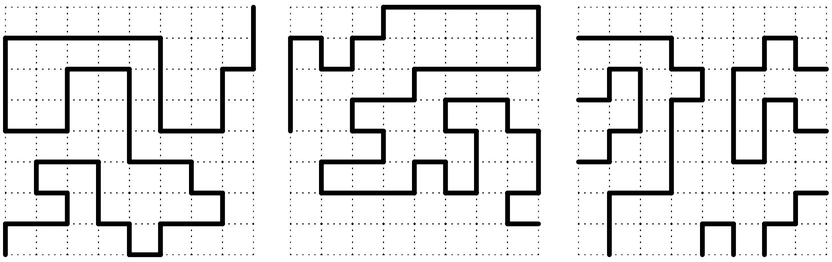

Figure 1. An example of a SAW configuration crossing a square (the left panel), traversing a square from left to right (the middle panel) and a cow-patch (the right panel).

anywhere on the left edge of the square and terminate anywhere on the right edge; so these are walks *traversing* the square from left to right. We call such walks *transverse* walks. Secondly, we consider the problem in which there may be several independent SAWs, each SAW starting and ending on the perimeter of the square. The SAWs are not allowed to take steps along the edges of the perimeter. Such walks partition the square into distinct regions and by colouring the regions alternately black and white we get a *cow-patch* pattern. Each problem is illustrated in figure 1.

Following the work in [18], Madras [13] proved a number of theorems. In fact, most of Madras's results were proved for the more general *d*-dimensional hyper-cubic lattice, but here we will quote them in the more restricted two-dimensional setting.

Theorem 1. *The following limits,*

$$\mu_1(x) := \lim_{L\to\infty} C_L(x)^{1/L} \qquad \text{and} \qquad \mu_2(x) := \lim_{L\to\infty} C_L(x)^{1/L^2},$$

are well defined in $\mathbb{R} \cup \{+\infty\}$.

More precisely,

(i) $\mu_1(x)$ *is finite for* $0 < x \leqslant 1/\mu$*, and is infinite for* $x > 1/\mu$*. Moreover,* $0 < \mu_1(x) < 1$ *for* $0 < x < 1/\mu$ *and* $\mu_1(1/\mu) = 1$.

(ii) $\mu_2(x)$ *is finite for all* $x > 0$*. Moreover,* $\mu_2(x) = 1$ *for* $0 < x \leqslant 1/\mu$ *and* $\mu_2(x) > 1$ *for* $x > 1/\mu$.

In [18] the existence of the limit $\mu_2(x)$ was proved, and in addition upper and lower bounds on $\mu_2(x)$ were established.

The average length of a (weighted) walk is defined to be

$$\langle n(x, L)\rangle := \sum_n n c_n(L) x^n \Big/ \sum_n c_n(L) x^n. \tag{5}$$

Theorem 2. *For* $0 < x < 1/\mu$*, we have that* $\langle n(x, L)\rangle = \Theta(L)$ *as* $L \to \infty$*, while for* $x > 1/\mu$*, we have* $\langle n(x, L)\rangle = \Theta(L^2)$.

In [18] it was proved that $\langle n(1, L)\rangle = \Theta(L^2)$. The situation at $x = 1/\mu$ is unknown. We provide compelling numerical evidence that in fact $\langle n(1/\mu, L)\rangle = \Theta(L^{1/\nu})$, where $\nu = 3/4$, in accordance with an intuitive suggestion in both [2] and [13].

Theorem 3. *For* $x > 0$*, define* $f_1(x) = \log \mu_1(x)$ *and* $f_2(x) = \log \mu_2(x)$.

(i) *The function* f_1 *is a strictly increasing, negative-valued convex function of* $\log x$ *for* $0 < x < 1/\mu$, *and* $f_1(x) = \Theta(-m(x))$ *as* $x \to 1/\mu^-$, *where* $m(x)$ *is the mass, defined by* (1).

(ii) *The function* f_2 *is a strictly increasing, convex function of* $\log x$ *for* $x > 1/\mu$, *and satisfies* $0 < f_2(x) \leqslant \log\mu + \log x$.

Some, but not all of the above results were previously proved in [18], but these three theorems elegantly capture all that is rigorously known.

The rest of the paper is organized as follows: In the next section we describe our enumeration methods, and explain how they are used to obtain radically extended series expansions for the number of walks crossing a square, the number of cow-patch configurations and the number of transverse SAWs. Section 3 details the results we have obtained. In section 4 we derive methods for obtaining rigorous upper and lower bounds on λ. In that section, we show that upper bounds based on counting cow-patch configurations are fully equivalent to the method of Abbott and Hanson, based on 0–1 admissible matrices. An improved method of lower bounds based on counting transverse walks is also derived. In section 5 we then apply these methods to our radically extended enumerations to provide significantly improved bounds on λ. In section 6 we give exact results for a short SAW crossing a square. The shortest SAW that can cross a square from $(0, 0)$ to (L, L) is of length $2L$. We give the exact number of such SAWs of length $2L + 2K$, for $K = 0, 1, 2$, and asymptotic results for $K = o(L^{1/3})$. Section 7 is devoted to a numerical analysis which gives precise (though non-rigorous) estimates of λ, for all three types of configurations, a discussion of the mean number of steps as a function of fugacity, fluctuations in this quantity, and a scaling theory for such fluctuations. We also speculate on the nature of the sub-dominant behaviour of the asymptotic form for the number of SAWs. Section 8 is also a numerical study, but of the number of SAWs that pass through the central vertex of an $L \times L$ square. Finally in section 9 we study Hamiltonian paths, obtaining both rigorous upper and lower bounds on the growth constant, and a numerical estimate.

2. Exact enumeration

In the following, we give a fairly detailed description of the algorithm we use to enumerate the number of walks crossing a square and briefly outline how this basic algorithm is modified in order to include a step fugacity, study SAWs traversing a square and the cow-patch configurations.

2.1. *The basic algorithm*

We use a transfer matrix algorithm to count the number of walks crossing $L \times M$ rectangles. The algorithm is based on the method of Conway *et al* [5] for enumerating ordinary self-avoiding walks. The transfer matrix technique involves drawing a boundary line through the rectangle intersecting $M + 1$ or $M + 2$ edges.

For each configuration of occupied or empty edges we maintain a count of partially completed walks intersecting the boundary in that pattern. Walks in rectangles are counted by moving the boundary adding one vertex at a time (see figure 2). Rectangles are built up column-by-column with each column constructed one vertex at a time. Configurations are represented by lists of states $\{\sigma_i\}$, where the value of the state σ_i at position i must indicate if the edge is occupied or empty. An empty edge is indicated by $\sigma_i = 0$. An occupied edge is either free (not connected to other edges) or connected to exactly one other edge via a path to

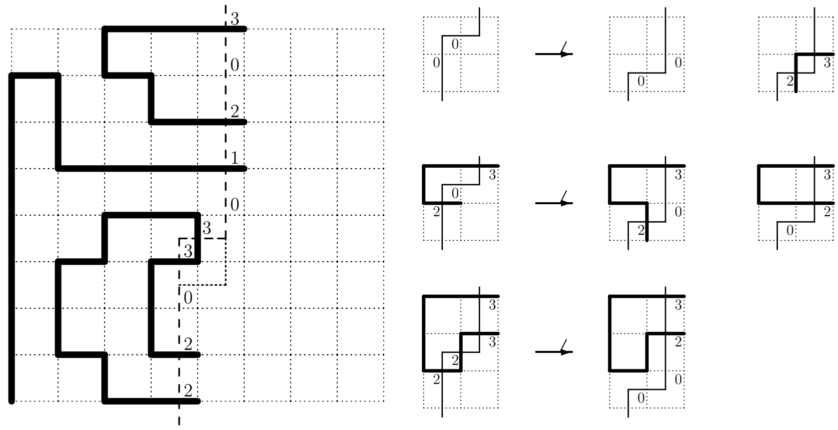

Figure 2. The left panel shows a snapshot of the intersection (the dashed line) during the transfer matrix calculation. Walks are enumerated by successive moves of the kink in the boundary, as exemplified by the position given by the dotted line, so that the $L \times M$ rectangle is built up one vertex at a time. To the left of the boundary we have drawn an example of a partially completed walk. Numbers along the boundary indicate the encoding of this particular configuration. The right panel shows some of the local configurations which occur as the kink in the intersection is moved one step.

Table 1. The various 'input' states and the 'output' states which arise as the boundary line is moved in order to include one more vertex. Each panel contains up to three possible 'output' states or other allowed actions.

Top / Bottom	0			1			2		3	
0	00	23		01	10	Res	02	20	03	30
1	01	10	Res				$\widehat{00}$	$\widehat{00}$		
2	02	20			$\widehat{00}$		$\overline{00}$			
3	03	30			$\widehat{00}$		00	$\overline{00}$		

the left of the boundary. We indicate this by $\sigma_i = 1$ for a free end, $\sigma_i = 2$ for the lower end of a loop and $\sigma_i = 3$ for the upper end of a loop connecting two edges. Since we are studying self-avoiding walks on a two-dimensional lattice the compact encoding given above uniquely specifies which ends are paired. Read from the bottom the configuration along the intersection in figure 2 is {2203301203} (prior to the move) and {2300001203} (after the move).

There are major restrictions on the possible configurations and their updating rules. Firstly, since the walk has to cross the rectangle there is exactly one free end in any configuration. Secondly, all remaining occupied edges are connected by a path to the left of the intersection and we cannot close a loop. It is therefore clear that the total number of 2s equals the total number of 3s. Furthermore, as we look through the configuration from the bottom the number of 2s is never smaller than the number of 3s (they are perfectly balanced parentheses). We also have to ensure that the graphs we construct have only one connected component. In the following, we shall briefly show how this is achieved.

We call the configuration before and after the move the 'source' and 'target', respectively. Initially, we have just one configuration with a single '1' at position 0 (all other entries '0') thus ensuring that we start in the bottom-left corner. As the boundary line is moved one step, we run through all the existing sources. Each source gives rise to one or two targets and the count of the source is added to the count of the target (the initial count of a target being zero).

After a source has been processed it can be discarded since it will make no further contribution. Table 1 lists the possible local 'input' states and the 'output' states which arise as the kink in the boundary is propagated one step and the various symbols will be explained below.

Firstly, the values of the 'Bottom' and 'Top' table entries refer to the edge states of the kink prior to the move. The Top (Bottom) entry is the state of the edge intersected by the horizontal (lower vertical) part of the boundary.

Some of the updating rules are illustrated further in figure 2. The top-most panels represent the input state '00' having the allowed output states '00' and '23' corresponding to leaving the edges empty or inserting a new loop, respectively. The middle panels represent the input state '20' with output states '20' and '02' from the two ways of continuing the loop end (note that the loop has to be continued since we would otherwise generate an additional free end not located at the allowed positions in the corners). The bottom-most panels represent the input state '22' as part of the configuration {02233}. In this case, we connect two loop ends and we thus join two separate loops into a single larger loop. The matching upper end of the innermost loop becomes the new lower end of the joined loop. The relabelling of the matching loop end when connecting two 2s (or two 3s) is denoted by overlining in table 1. When we join loop ends to a free end (inputs '12', '21', '13' and '31') we have to relabel the matching loop end as a free end. This type of relabelling is indicated by the symbol $\widehat{00}$. The input state '11' never occurs since there is only one free end. The input state '23' is not allowed since connecting the two ends results in a closed loop and we thus discard any configuration in which a closed loop is formed. It is quite easy to avoid forming closed loops. We only have to be careful when the input is '03' or '30'. If the upper end of the loop is continued along the vertical output edge we would form a closed loop if the horizontal edge immediately below was a lower loop end, and we just check the state of this edge and only proceed if it is not in state '2' (naturally the upper loop end can always be continued along the horizontal output edge).

Finally, we have marked two outputs, from the inputs '01' and '10' with 'Res', indicating situations where we terminate free ends. This results in completed partial walks and is only allowed if there are no other occupied edges in the source (otherwise we would produce graphs with separate pieces) and if we are at the top-most vertex (otherwise we would not cross the rectangle). The count for this configuration is the number of walks crossing a rectangle of height M and length L equal to the number of completed columns.

The time required to obtain the number of walks on $L \times M$ rectangles grows exponentially with M and linearly with L. Time and memory requirements are basically proportional to the maximal number of distinct configurations along the boundary line. When there is no kink in the intersection (a column has just been completed) we can calculate this number, $N_{\mathrm{conf}}(M)$, exactly. Obviously, the free end cuts the boundary line configuration into two separate pieces. Each of these pieces consists of 0s and an equal number of 2s and 3s with the latter forming a perfectly balanced parenthesis system.

Each piece thus corresponds to a Motzkin path [17, chapter 6] (just map 0 to a horizontal step, 2 to a north-east step, and 3 to a south-east step). The number of Motzkin paths M_n with n steps is easily derived from the generating function $\mathcal{M}(x) = \sum_n M_n x^n$, which satisfies $\mathcal{M} = 1 + x\mathcal{M} + x^2\mathcal{M}^2$, so that

$$\mathcal{M}(x) = \left[1 - x - \sqrt{(1+x)(1-3x)}\,\right]\big/2x^2. \tag{6}$$

The number of configurations $N_{\mathrm{conf}}(M)$ for a rectangle of height M is simply obtained by inserting a free end between two Motzkin paths, so that the generating function $\sum_M N_{\mathrm{conf}}(M)x^M$ is simply $x\mathcal{M}(x)^2$. The Lagrange inversion formula gives

$$N_{\mathrm{conf}}(M) = 2\sum_{i\geqslant 0} \frac{(M+1)!}{i!(i+2)!(M-2i)!}.$$

When the boundary line has a kink the number of configurations exceeds $N_{\mathrm{conf}}(M)$ but clearly is less than $N_{\mathrm{conf}}(M+1)$. From (6) we see that asymptotically $N_{\mathrm{conf}}(M)$ grows like 3^M (up to a power of M). So the same is true for the maximal number of boundary line configurations and hence for the computational complexity of the algorithm. Note that the total number of walks grows like λ^{LM}, so our algorithm leads to a better than exponential improvement over direct enumeration.

The integers occurring in the expansion become very large so the calculation was performed using modular arithmetic [11]. This involves performing the calculation modulo various prime numbers p_i and then reconstructing the full integer coefficients at the end. We used primes of the form $p_i = 2^{30} - r_i$ where r_i are distinct integers, less than 1000, such that p_i is a (different) prime for each value of i. The Chinese remainder theorem ensures that any integer has a unique representation in terms of residues. If the largest integer occurring in the final expansion is m, then we have to use a number of primes k such that $p_1 p_2 \cdots p_k > m$.

2.2. Extensions of the algorithm

The algorithm is easily generalized to include a step fugacity x. The count associated with the boundary line configuration has to be replaced by a generating function for partial walks. Since we only use this generalization to study walks crossing an $L \times L$ square the generating function is just a polynomial of degree (at most) $L(L+2)$ in x. The coefficient of x^n is just the number of partial walks of length n intersecting the boundary line in the pattern specified by the configuration. The generating function of the source is multiplied by x^m and added to the target, where m is the number of additional steps inserted. Not all $L(L+2)$ terms in the polynomials need be retained. Firstly, any walk crossing the square has even length. Thus in the generating functions for partial walks either all the even or all the odd terms are zero, and we need only retain the non-zero terms. Secondly, in order to construct a given boundary line configuration, a certain minimal number of steps n_{min} are required. Terms in the generating function of degree lower than n_{min} are therefore zero and again we need not store these.

The generalization to traversing walks is also quite simple. Firstly, we have $M+1$ initial configurations which are empty except for a free end at position $0 \leqslant j \leqslant M$. This corresponds to the $M+1$ possible starting positions for the walk on the left boundary. Secondly, we have to change how we produce the final counts. The easiest way to ensure that a walk spans the rectangle and that only single component graphs are counted is as follows: when column $L+1$ has been completed we look at the $M+1$ configurations with a single free end and add the counts from all of them. This is the number of walks traversing an $L \times M$ rectangle.

The generalization to cow-patch patterns is more complicated. Graphs can now have many separate components each of which is a SAW, and there can thus be many free ends in a boundary line configuration. Note that each SAW starts and terminates with a step perpendicular to the border of the rectangle and there are never any steps along the edges of the borders of the rectangle. There are 2^{M-1} initial configurations since any of the edges in the first column from position 1 to $M-1$ can be occupied by a free end or be empty (recall that in cow-patch configurations the top- and bottom-most horizontal edges cannot be occupied). There is an extra updating rule in the bulk in that we can have the local input '11' (joining of two free ends) with the only possible output being '00'. Also the updating rules at the upper and lower borders of the rectangle are different in this case. At the upper border we only have the input '00' with the outputs '00' and '10' corresponding to the insertion of a free end on a vertical edge at the upper border. There are no '23' or '01' outputs since these would produce an occupied edge along the upper border. At the lower border we have inputs '00', '01' and '02' and in each case the only possible output is '00' (with the appropriate relabelling in the

'02' case). Finally, the count of the number of cow-patch patterns is obtained by summing over all boundary line configurations after the completion of a column.

3. Results

As discussed above, in order to obtain the exact value of the number of SAWs crossing a square, some of which are integers with nearly 100 digits, we performed the enumerations several times, each time *modulo* a different prime. The enumerations were then reconstructed using the Chinese remainder theorem. Each run for a 19×19 lattice took about 72 h using eight processors of a multiprocessor 1 GHz Compaq Alpha computer. Ten such runs were needed to uniquely specify the resultant numbers.

Proceeding as above, we have calculated $c_n(L)$ for all n for $L \leqslant 17$. In other words, we have obtained the polynomials $C_L(x)$ for $L \leqslant 17$. In addition, we have computed $C_{18}(1)$ and $C_{19}(1)$, the total number of SAWs crossing an 18×18 and 19×19 square, respectively. We have also computed the corresponding quantities for cow-patch and transverse SAWs, denoted as $P_L(1)$ and $T_L(1)$ respectively, for $L \leqslant 19$. These are given in table 2.

In [1] the question was asked whether $C_{L,M}^{\frac{1}{LM}}$ is decreasing in both L and M. We can answer this in the negative, based on our enumerations.

4. Proofs of bounds

Let $\mathcal{C}(L)$ be the set of self-avoiding walks crossing the $L \times L$ square from its south-west corner $(0, 0)$ to its north-east corner (L, L). Let $C(L)$ denote the cardinality of $\mathcal{C}(L)$. Let $\mathcal{T}(L)$ be the set of self-avoiding walks that *traverse*, the $L \times L$ square: by this, we mean that the walk starts from the west edge of the square and ends on the east edge (figure 1). Let $T(L)$ be the cardinality of $\mathcal{T}(L)$. Finally, let $\mathcal{P}(L)$ be the set of *cow-patches*, of size L: a *cow-patch* is a configuration of mutually avoiding self-avoiding walks on the $L \times L$ square, such that each walk has both endpoints on the border of the square, but never contains an edge of the border (figure 1). Let $P(L)$ be the number of cow-patches of size L.

We first prove in this section that

$$\lim C(L)^{1/L^2} = \lim T(L)^{1/L^2} = \lim P(L)^{1/L^2} = \lambda. \tag{7}$$

Then, we prove the following bounds on λ: for $L \geqslant 1$,

$$C(L)^{1/(L+1)^2} \leqslant \lambda, \qquad T(L)^{1/((L+1)(L+2))} \leqslant \lambda, \qquad \lambda \leqslant (2P(L))^{1/L^2}.$$

Let us first focus on (7). As recalled in the previous sections, the convergence of $C(L)^{1/L^2}$ to λ has been proved in earlier papers [1, 18]. For walks of $\mathcal{T}(L)$, a similar result follows from the fact that

$$C(L) \leqslant T(L) \leqslant C(L+2).$$

The first inequality above is obvious. The second one is explained on the left of figure 3.

For cow-patches, the existence and value of $\lim P(L)^{1/L^2}$ follow from

$$C(L-1) \leqslant P(L) \leqslant C(L+3).$$

The first inequality is explained on the right of figure 3. The second one is a bit more tricky. We borrow the following argument from [7]. It is illustrated in figure 4. Start from a cow-patch of size L. Colour all cells of the square in black and white, in such a way that the south-west corner of the square is black and each step included in one of the walks of the cow-patch is adjacent to a black cell and a white one. Surround the square by a layer of black cells, so as

Table 2. The total number of walks crossing a square, $C_L(1)$, cow-patch walks, $P_L(1)$ and traversing walks, $T_L(1)$.

L	$C_L(1)$
1	2
2	12
3	184
4	8 512
5	1 262 816
6	575 780 564
7	789 360 053 252
8	3 266 598 486 981 642
9	41 044 208 702 632 496 804
10	1 568 758 030 464 750 013 214 100
11	182 413 291 514 248 049 241 470 885 236
12	64 528 039 343 270 018 963 357 185 158 482 118
13	69 450 664 761 521 361 664 274 701 548 907 358 996 488
14	227 449 714 676 812 739 631 826 459 327 989 863 387 613 323 440
15	2 266 745 568 862 672 746 374 567 396 713 098 934 866 324 885 408 319 028
16	68 745 445 609 149 931 587 631 563 132 489 232 824 587 945 968 099 457 285 419 306
17	6 344 814 611 237 963 971 310 297 540 795 524 400 449 443 986 866 480 693 646 369 387 855 336
18	1 782 112 840 842 065 129 893 384 946 652 325 275 167 838 065 704 767 655 931 452 474 605 826 692 782 532
19	1 523 344 971 704 879 993 080 742 810 319 229 690 899 454 255 323 294 555 776 029 866 737 355 060 592 877 569 255 844
L	**$\frac{1}{2} P_L(1)$**
1	1
2	7
3	160
4	11 408
5	2 522 191
6	1 718 769 373
7	3 598 611 604 598
8	23 098 353 998 190 640
9	453 839 082 673 896 579 243
10	27 266 319 759 961 440 667 165 921
11	5 005 013 940 387 988 257 218 110 301 496
12	2 805 250 606 288 167 736 619 664 411 164 848 668
13	4 798 636 658 841 347 169 993 094 278 185 741 344 065 154
14	25 042 563 713 780 942 969 666 110 695 844 976 426 050 692 260 400
15	398 585 071 868 378 544 875 200 967 972 920 693 215 965 420 927 547 891 443
16	19 343 509 060 397 504 009 184 634 223 201 418 820 841 655 935 064 055 180 184 148 711
17	2 861 743 739 297 615 012 905 209 591 294 651 941 414 000 218 185 488 280 077 237 678 797 763 881
18	1 290 420 684 731 131 093 964 422 300 362 403 673 911 432 011 198 730 662 653 676 329 480 448 243 238 167 005
19	1 773 260 101 104 126 884 305 729 846 781 529 391 070 539 884 533 101 171 392 023 893 295 633 931 250 883 380 602 647 575
L	**$T_L(1)$**
1	8
2	95
3	2 320
4	154 259
5	30 549 774
6	17 777 600 753
7	30 283 708 455 564
8	152 480 475 641 255 213
9	2 287 842 813 828 061 810 244

Table 2. (Continued.)

L	$T_L(1)$
10	102 744 826 737 618 542 833 764 649
11	13 848 270 995 235 582 268 846 758 977 770
12	5 613 766 870 113 075 134 552 249 300 590 982 081
13	6 856 324 633 418 315 229 580 098 999 727 214 234 534 626
14	25 264 653 780 547 704 599 613 926 971 040 640 439 380 254 497 299
15	281 194 924 965 510 769 640 501 069 703 642 937 039 678 809 002 355 743 600
16	9 461 739 046 646 537 749 639 494 171 503 923 182 753 987 897 972 167 546 351 180 871
17	963 236 702 020 101 408 274 810 653 629 921 860 636 656 580 683 490 560 257 709 270 360 444 788
18	296 872 411 379 358 777 499 142 156 584 947 972 393 781 613 934 413 706 389 772 635 139 720 532 797 697 401
19	277 150 300 263 332 125 727 926 989 254 635 730 407 844 207 233 646 123 561 354 535 935 393 720 183 262 709 640 734 296

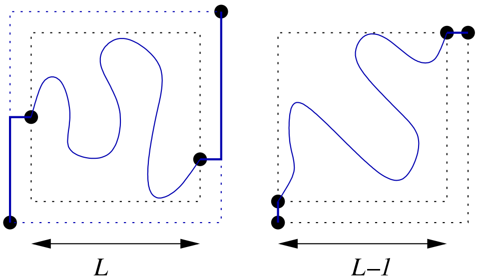

Figure 3. From transverse walks to walks crossing a square (left). From walks crossing a square to cow-patches (right).

to obtain a square of size $L+2$, containing a certain number of white regions. For *each* white region, dig a tunnel (exactly one tunnel) in the outer layer to connect it to the outer world. In the figure thus obtained, the border of the black region forms a self-avoiding *polygon*, that includes each walk of the cow-patch. It remains to extend this polygon in a canonical way to obtain a walk of $\mathcal{C}(L+3)$, illustrated in the last panel of figure 4.

Let us now discuss lower and upper bounds on λ. The left-hand side of figure 5 shows that for all ℓ and all odd k, it is possible to combine k^2 elements of $\mathcal{C}(\ell)$ to form an element of $\mathcal{C}(L)$ with $L = k(\ell+1)$. In figure 5, $k = 3$. This shows that

$$C(\ell)^{k^2} \leqslant C(L).$$

Hence

$$C(\ell)^{1/(\ell+1)^2} \leqslant C(L)^{1/L^2}.$$

Taking the limit as $k \to \infty$ implies that for all ℓ,

$$C(\ell)^{1/(\ell+1)^2} \leqslant \lambda.$$

Similarly, let us try to pack transverse walks densely. The right-hand side of figure 5 shows that for all ℓ and k, it is possible to combine $k^2(\ell+1)(\ell+2)$ elements of $\mathcal{T}(\ell)$ to form an element of $\mathcal{C}(L)$ with $L = k(\ell+1)(\ell+2)$. This shows that

$$T(\ell)^{k^2(\ell+1)(\ell+2)} \leqslant C(L).$$

Hence

$$T(\ell)^{1/((\ell+1)(\ell+2))} \leqslant C(L)^{1/L^2}.$$

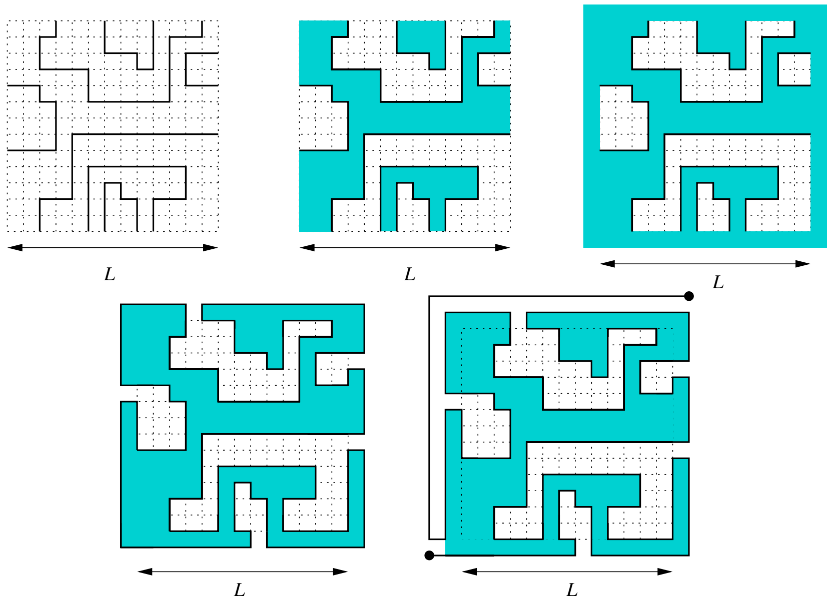

Figure 4. From cow-patches to walks crossing a square.

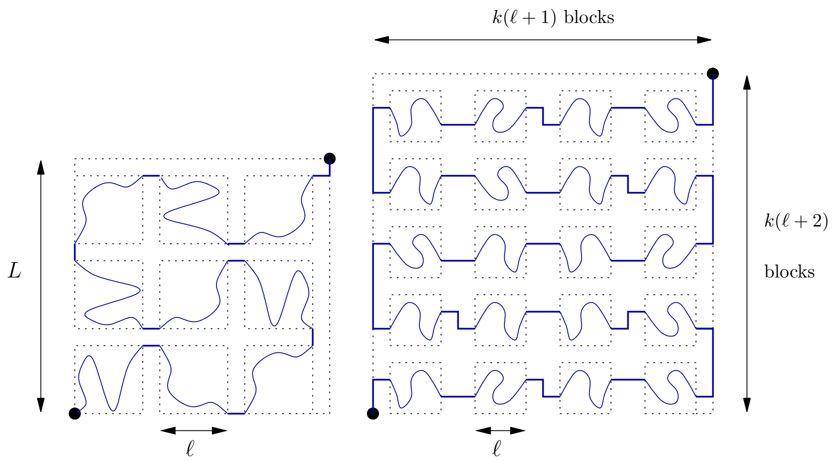

Figure 5. Dense packings of walks crossing or traversing a square.

Taking the limit as $k \to \infty$ implies that for all ℓ,

$$\lambda \geqslant T(\ell)^{1/((\ell+1)(\ell+2))}. \tag{8}$$

Let us finally give upper bounds for λ. Define a coloured cow-patch as a cow-patch in which the various regions are coloured in black and white, in such a way that two adjacent regions have different colours. Clearly, each cow-patch gives rise to 2 coloured cow-patches. Observe that there is a bijection between coloured cow-patches of size L and the *admissible*, matrices of the same size, as defined in section 5. Since an element of $\mathcal{C}(L)$, with $L = k\ell$, can be seen as the juxtaposition of k^2 admissible matrices (or coloured cow-patches) of size ℓ,

$$C(L) \leqslant (2P(\ell))^{k^2}.$$

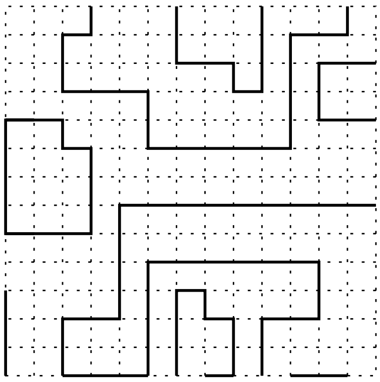

Figure 6. A generalized cow-patch.

That is,

$$C(L)^{1/L^2} \leqslant (2P(\ell))^{1/\ell^2}$$

and by letting $k \to \infty$, we obtain Abbott and Hanson's bound: for all ℓ,

$$\lambda \leqslant (2P(\ell))^{1/\ell^2}.$$

One possible attempt to improve this bound is to consider *generalized* cow-patches, in which the walks are allowed to include edges lying on the west and south borders of the square (figure 6). Let $GP(L)$ denote the number of generalized cow-patches of size L. Since an element of $\mathcal{C}(L)$, with $L = k\ell$, can be seen as the juxtaposition of k^2 generalized patches, the above argument gives

$$\lambda \leqslant GP(\ell)^{1/\ell^2}.$$

We have not exploited this improvement, as it only changes the fourth significant digit of our bound.

5. Bounds on the growth constant λ

For the more general problem of SAW going from (0, 0) to (L, M) on an $L \times M$ lattice, it was proved in [1] that

Theorem 4. *For each fixed M, $\lim_{L\to\infty} C_{L,M}^{\frac{1}{LM}} = \lambda_M$ exists.*

Further, Abbott and Hanson state that a similar proof can be used to establish that $\lim_{L\to\infty} C_{L,L}^{\frac{1}{L^2}} := \lambda$ exists. This was proved rather differently in [18].

5.1. Upper bounds on λ

In [1] an upper bound on the growth constant λ was obtained by recasting the problem in a matrix setting. We give below an alternative method for establishing upper bounds, based on defining a superset of paths. We then show that these two methods are in fact identical.

Following [1], consider any non-intersecting path crossing the $L \times L$ square. Label each unit square in the $L \times L$ lattice by 1 if it lies to the right of the path, and by 0 if it lies to the left. This provides a one-to-one correspondence between paths and a subset of $L \times L$ matrices with elements 0 or 1. Matrices corresponding to allowed paths are called *admissible*, otherwise they are *inadmissible*. Since the total number of $L \times L$ 0–1 matrices is 2^{L^2}, we immediately have the weak bound $C_{L,L} \leqslant 2^{L^2}$. Of the 16 possible 2×2 matrices, only 14 can correspond to portions of non-intersecting lattice paths. Note that there are only 12 actual paths from (0, 0) to (2, 2), but a further two matrices may correspond to paths that are embedded in a larger lattice. Thus we find the bound $C_{L,L} \leqslant 14^{(L/2)^2}$, so $\lambda \leqslant 1.9343\ldots$ Similarly, for 3×3 lattices we find 320 admissible matrices (out of a possible 512), so $\lambda \leqslant 320^{1/9} = 1.8982\ldots$. For 4×4 lattices, [1] claims that there are 22 662 admissible matrices, but we believe the correct number to be 22 816, giving the bound $\lambda \leqslant 1.8723\ldots$. We have made dramatic extensions of this work, using a combination of finite-lattice methods and transfer matrices, as described below, and have determined the number of admissible matrices up to 19×19. There are $3.546\,5202\ldots \times 10^{90}$ such matrices, giving the bound

$$\lambda \leqslant 1.7817.$$

This bound is fully equivalent to the bound $\lambda \leqslant (2P_L)^{1/L^2}$, where P_L denotes the number of cow-patch configurations on the $L \times L$ lattice. This bound was proved in section 4, and the equivalence follows upon colouring cow-patches by two colours, such that adjacent regions have different colours. Labelling the two colours 0 and 1 produces a 0–1 matrix representation.

5.2. Lower bounds on λ

In [1] the useful bound

$$\lambda > \lambda_M^{\frac{M}{M+1}} \tag{9}$$

is proved.

The above evaluation of λ_2, see (4), immediately yields $\lambda > 1.4892\ldots$.

Based on exact enumeration, we have found the exact generating functions $G_M(z) = \sum_L C_{L,M} z^L$ for $M \leqslant 6$. For $M = 3$ we find

$$G_3(z) = \frac{[1, -4, -4, 36, -39, -26, 50, 6, -15, 1]}{[1, -12, 54, -124, 133, 16, -175, 94, 69, -40, -12, 4, 1]},$$

where we denote by $[a_0, a_1, \ldots, a_n]$ the polynomial $a_0 + a_1 z + \cdots + a_n z^n$. As explained above, all the generating functions $G_M(z)$ are rational. For $M = 4, 5, 6$, their numerator and denominators are found to have degree (26, 27), (71, 75) and (186, 186) respectively, in an obvious notation.

From these, we find the following values: $\lambda_3 = 1.763\,31\ldots$, $\lambda_4 = 1.751\,46\ldots$, $\lambda_5 = 1.748\,75\ldots$ and $\lambda_6 = 1.747\,28\ldots$. Then from equation (9) and λ_6 we obtain the bound $\lambda > 1.613\,39\ldots$.

However, an alternative lower bound can be obtained from transverse SAWs, defined in section 1. If T_L denotes the number of transverse SAWs on the $L \times L$ lattice, then we proved in the previous section that

$$\lambda \geqslant T(L)^{1/((L+1)(L+2))}. \tag{10}$$

From our enumerations of $T(L)$, given above for $L \leqslant 19$, we obtain the improved bound $\lambda > 1.6284$.

Combining our results for lower and upper bounds finally gives

$$1.6284 < \lambda < 1.7817.$$

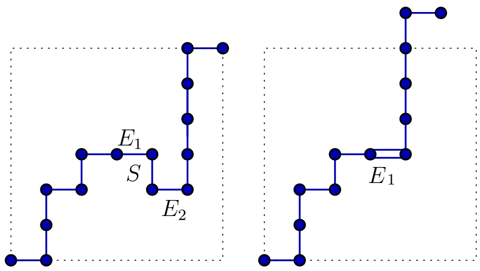

Figure 7. Enumeration of self-avoiding walks with one vertical defect.

6. Short walks crossing a square

As defined in the introduction, let $c_n(L)$ be the number of n-step self-avoiding walks crossing an $L \times L$ square. Clearly, this number is zero when n is odd and also when $n < 2L$. It is almost as clear that

$$c_{2L}(L) = \binom{2L}{L}.$$

Indeed, there are $2L$ steps in the path, of which L must go north and L must go east. Note that the number $c_{2L}(L)$ has asymptotic expansion

$$\frac{4^L}{\sqrt{L\pi}}\left(1 - \frac{1}{4L} + \frac{1}{128L^2} + \frac{5}{1024L^3} + \cdots\right).$$

Let us now prove that

$$c_{2L+2}(L) = 2L\binom{2L}{L-2}.$$

A walk counted by $c_{2L+2}(L)$ has either $L+2$ vertical steps (and L horizontal ones), or L vertical steps (and $L+2$ horizontal ones). By symmetry, we can focus on the first case. Let w be such a walk. We say that w has a *vertical* defect. Among the $L+2$ vertical steps of w, exactly one goes south, while the $L+1$ others go north. The unique south step S is necessarily preceded and followed by an east step, which we denote respectively by E_1 and E_2. Let us mark E_1 and delete S and E_2 (figure 7). The marked path w' thus obtained allows one to recover the original path w. It contains $L+1$ north steps and $L-1$ east steps, one of which is marked. Moreover, the marked step cannot be at ordinate 0, nor at ordinate $L+1$. Conversely, any walk w' satisfying these properties is obtained (exactly once) from a walk counted by $c_{2L+2}(L)$ and having a vertical defect.

The number of walks having $L+1$ north steps and $L-1$ east steps is $\binom{2L}{L-1}$. Marking one of the east steps gives a factor $(L-1)$. Now we must subtract the number of walks in which the marked step is either at level 0 or at level $N+1$. Transforming the marked step into a vertical step shows that each of these two families of marked walks is in bijection with walks formed with $L+2$ up steps and $L-2$ down steps. Putting these observations together gives

$$c_{2L+2}(L) = 2\left((L-1)\binom{2L}{L-1} - 2\binom{2L}{L-2}\right) = 2L\binom{2L}{L-2}.$$

Note that the number $c_{2L+2}(L)$ has the asymptotic expansion

$$\frac{L4^L}{\sqrt{L\pi}}\left(2 - \frac{33}{4L} + \frac{1345}{64L^2} - \frac{238\,35}{512L^3} + \cdots\right).$$

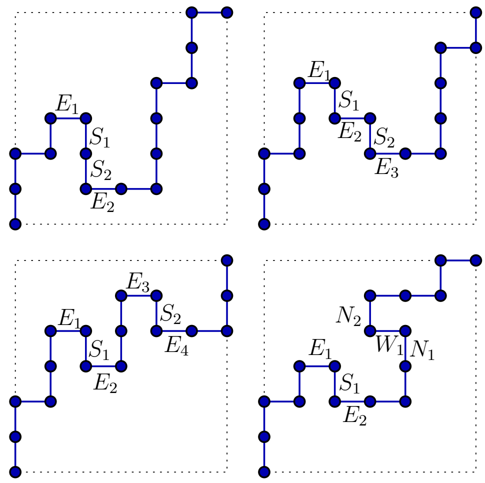

Figure 8. Four types of self-avoiding walks with two defects.

The same ideas may be used to find the value of $c_{2L+4}(L)$. We will prove that

$$\frac{1}{2}c_{2L+4}(L) = \frac{(2L)!}{L!(L+4)!}(48 + 90L + 8L^2 - 28L^3 - 3L^4 + 4L^5 + L^6) - 2. \tag{11}$$

First, note that $c_{2L+4}(L)/2$ is the number of self-avoiding walks (of length $2L + 4$, crossing the $L \times L$ square) in which the first defect, that is, the first *backward* step, is a south step. We focus on such walks, and study four distinct cases. The first three cases count walks having two south steps, and the last case count walks having a south step and a west step (figure 8).

(i) The walk w contains two adjacent south steps, S_1 and S_2. They are necessarily preceded by an east step E_1, and followed by another east step E_2. The walk has $L + 4$ vertical steps and L horizontal steps. Mark E_1, and delete S_1, S_2, E_2 in order to obtain a walk w' with $L + 2$ north steps and $L - 1$ east steps, one of which is marked. In w', the marked step cannot be at level 0, 1, $L+1$ or $L+2$. Using the same ingredients as above, we obtain the number of such walks as

$$(L-1)\binom{2L+1}{L-1} - 4\binom{2L+1}{L-2}.$$

(ii) The walk contains a sequence $E_1S_1E_2S_2E_3$. Again, w has $L + 4$ vertical steps and L horizontal steps. Mark E_1, and delete S_1, E_2, S_2 and E_3 in order to obtain a walk with $L + 2$ north steps and $L - 2$ east steps, one of which is marked. In w', the marked step cannot be at level 0, 1, $L + 1$ or $L + 2$. The number of such walks is

$$(L-2)\binom{2L}{L-2} - 4\binom{2L}{L-3}.$$

(iii) The walk contains a sequence $E_1S_1E_2$, and, further away, another sequence $E_3S_2E_4$, disjoint from the first one. Again, w has $L+4$ vertical steps and L horizontal steps. Mark the steps E_1 and E_3, delete S_1, E_2, S_2 and E_4 in order to obtain a walk with $L + 2$ north steps and $L - 2$ east steps, two of which are marked. Note that, in w', the first marked step cannot lie at level 0, $L + 1$ or $L + 2$, while the second marked step cannot lie at level 0, 1 or $L + 2$. Using the same ingredients as above, combined with the inclusion–exclusion principle, we find the number of such walks as

$$\binom{L-2}{2}\binom{2L}{L-2} - 2\left[(L-3)\binom{2L}{L-3} - \binom{2L}{L-4}\right] - 4\binom{2L}{L-4} - 2\binom{2L}{L-4} + 5\binom{2L}{L-4} = \binom{L-2}{2}\binom{2L}{L-2} - 2(L-3)\binom{2L}{L-3} + \binom{2L}{L-4}.$$

(iv) The walk w contains a sequence $E_1S_1E_2$, and, further away, a sequence $N_1W_1N_2$ (with obvious notation). It thus contains $L+2$ vertical steps and $L+2$ horizontal ones. Mark the steps E_1 and N_1, delete S_1, E_2, W_1 and N_2 in order to obtain a walk w' with L north steps and L east steps, in which one step of each type is marked in such a way that the east marked step comes before the north marked step. In w', the two marked steps cannot be consecutive (or w would not be self-avoiding), the east marked step cannot lie at level 0, and the north marked step cannot lie at abscissa L. Again, the inclusion–exclusion principle applies and gives the number of such walks as

$$\frac{1}{2}L^2\binom{2L}{L} - (2L-1)\binom{2L-2}{L-1} - 2L\binom{2L}{L-1} + 2\binom{2L-1}{L-1} + \left[\binom{2L}{L} - 1\right] - 1.$$

Putting together the four partial results we have obtained gives (11). Note that the number $c_{2L+4}(L)$ has the asymptotic expansion

$$\frac{L^2 4^L}{\sqrt{L\pi}}\left(2 - \frac{49}{4L} + \frac{2913}{64L^2} - \frac{92971}{512L^3} + \cdots\right).$$

The above argument suggests that it is very likely that, for every fixed K, the sequence $c_{2L+2K}(L)$, for $L \geqslant 0$, is *polynomially recursive* [16, 17, chapter 6].

While it would probably be possible to find the number of possible paths of length $2L+6$, the number of special cases that must be treated would become onerous. We have therefore resorted to a numerical study for walks of length $2L+2K$, $K > 2$, based on our enumerations. For $K = 3$ we found

$$\frac{L^3 4^L}{\sqrt{L\pi}}\left(\frac{4}{3} - \frac{49}{6L} + \frac{1931 \pm 1}{64L^2} + \cdots\right),$$

while the corresponding result for $K = 4$ is

$$\frac{L^4 4^L}{\sqrt{L\pi}}\left(\frac{2}{3} + \frac{11}{4L} + \cdots\right).$$

We can give a heuristic argument for the general form of the leading term in the asymptotic expansion of the number of walks of length $2L+2K$ which gives as the leading order term $\frac{4^L}{\sqrt{L\pi}}\frac{(2L)^K}{K!}$. Here the first factor is given by the number of ways of choosing the backbone, $\binom{2L}{L} \sim \frac{4^L}{\sqrt{L\pi}}$ and the second is given by the number of ways of placing K defects (or backward steps) on a path of length $2L$, which is just $(2L)^K$. The defects are indistinguishable, introducing the factor $K!$.

This argument can be refined into a proof, for $K = \mathrm{o}(L^{1/3})$ by following the steps, *mutatis mutandis* in the proof of a similar result given in [8].

7. Numerical analysis

It has been proved [1, 18] that $\lim_{L\to\infty} C_{L,L}^{\frac{1}{L^2}} = \lambda$ exists. From this it is likely that $R_L = C_{L+1,L+1}/C_{L,L} \sim \lambda^{2L}$ though this has not been proved. Accepting this, the generating function $\mathcal{R}(x) = \sum_L R_L x^L$ will have the radius of convergence $x_c = 1/\lambda^2$, which we can estimate accurately using differential approximants [9]. In this way, we estimate that for the crossing problem $x_c = 0.328\,58(5)$, for the transverse problem $x_c = 0.3282(6)$ and for the cow-patch problem $x_c = 0.328\,574(2)$. It is reassuring to see, from our numerical studies, that λ appears to be the same for the three problems, as proved above, and we estimate that $\lambda = 1.744\,550(5)$.

We now speculate on the sub-dominant terms. For SAW on an infinite lattice, it is widely accepted that $c_n \sim \text{const}\,\mu^n n^g$ where c_n is the number of n-step SAWs equivalent up to a translation.

It seems at least a plausible speculation that, for a SAW crossing an $L \times L$ lattice, the number going from $(0, 0)$ to (L, L) is given by $\sim A\lambda^{L^2+bL}L^{\alpha}$. We have investigated this possibility numerically, and found it to be supported by the data, to some extent.

We fitted the data to the assumed form, fixing the value of λ at our best estimate, 1.744 550. This then leaves two unknown parameters b and α. For cow-patch walks we find $b \approx 0.8558$ and $\alpha \approx -0.500$. This suggests asymptotic behaviour $A_P\lambda^{L^2+0.8558L}/\sqrt{L}$, and we estimate $A_P \approx 0.52$. For transverse walks and walks crossing a square b is quite small, most likely zero. A value of $b = 0$ would imply the absence of a term $\mathrm{O}(\lambda^{bL})$, or possibly the presence of a term $\mathrm{O}(\log L)$, or some power of a logarithm. We have investigated the latter possibility by including a logarithmic factor, and found that the data do not support the presence of such a term for either class of walk. Of course, we cannot rule out some small power of a logarithm, but this seems less likely than the absence of a term $\mathrm{O}(\lambda^{bL})$.

We next investigated the possibility that the sub-dominant term is $\mathrm{O}(L^{\alpha})$. A simple ratio analysis [9] then led to the estimates $\alpha = -0.7$ for walks crossing a square, and $\alpha = 1.0$ for transverse walks. If our assumed form is correct, we expect these estimates to be accurate to within 10–15%. We also studied the sequence whose terms are given by the quotient T_L/C_L. This has the advantage that the λ dependence cancels, and so our result is independent of any uncertainty in the value of λ. We find that $T_L/C_L \sim \text{const}\,L^{1.7}$ This is in agreement with the estimates of α found separately, for the two series. Thus we very tentatively speculate that $C_L \sim 8\lambda^{L^2}/L^{0.7}$ and $T_L \sim 9\lambda^{L^2}L$, where the amplitude estimates follow by the simple expedient of fitting the assumed L-dependent form to the data, term-by-term, and extrapolating the resulting sequence of amplitude estimates. Given the sensitivity of the amplitudes to both λ and α, we do not feel confident quoting an uncertainty for the amplitudes.

Whittington and Guttmann [18] and later Burkhardt and Guim [2] studied the behaviour of the mean number of steps in a path on an $L \times L$ lattice

$$\langle n(x, L)\rangle = \frac{\sum_n n c_n(L)x^n}{\sum_n c_n(L)x^n} \tag{12}$$

as well as the fluctuations of this quantity

$$V(x, L) = \frac{\sum_n n^2 c_n(L)x^n}{\sum_n c_n(L)x^n} - \langle n(x, L)\rangle^2 \tag{13}$$

which is a kind of heat capacity. As discussed above, a phase transition takes place as one varies the fugacity x associated with the walk length. At a critical value x_c, the average walk length of a path on an $L \times L$ lattice changes from $\Theta(L)$ to $\Theta(L^2)$. In [18] the critical fugacity was proved to satisfy $1/\mu \leqslant x_c \leqslant \mu_H$, where μ_H is the growth constant for a Hamiltonian SAW on the square lattice, and on the basis of numerical studies conjectured to be $x_c = 1/\mu$ exactly. In [13] the conjecture was proved. Here we also study the behaviour at $x = x_c$ and find that $\langle n(x, L)\rangle = \Theta(L^{1/\nu})$ where the numerical evidence is consistent with $\nu = 3/4$. Similar conclusions were reached earlier in [2]. For any given value of L the fluctuation $V(x, L)$ is observed to have a single maximum located at $x_c(L)$ (see the top-left panel of figure 9). We study in detail the behaviour of $V(x, L)$, which we expect to obey a standard

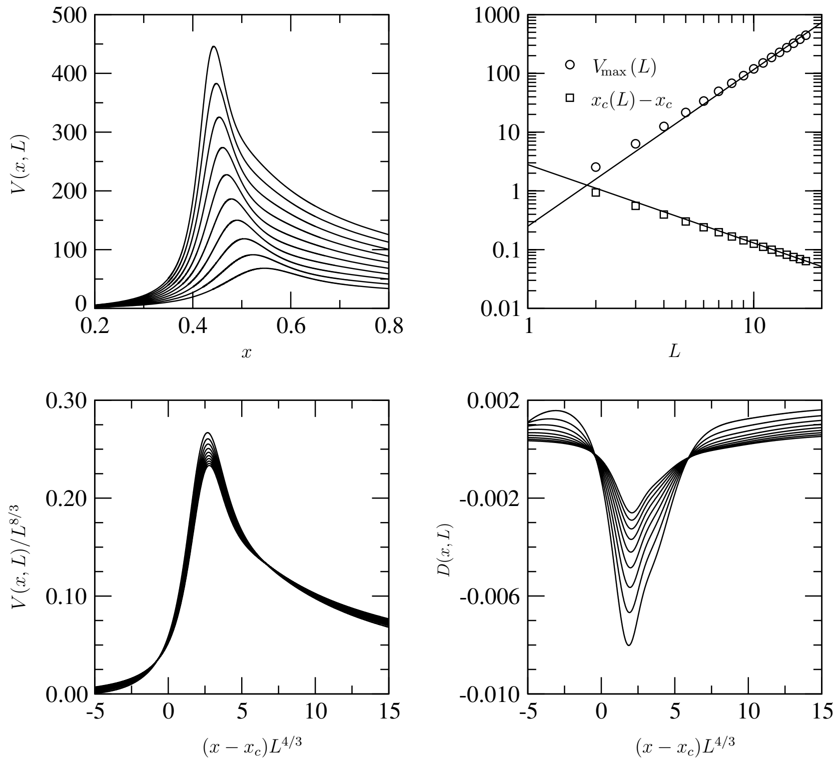

Figure 9. The fluctuations $V(x, L)$ as a function of the fugacity x (the top-left panel). $x_c(L) - x_c$ and $V_{\max}$ versus L (the top-right panel). $V(x, L)/L^{8/3}$ (the bottom-left panel) and $D(x, L)$ (the bottom-right panel) versus the scaling variable $(x - x_c)L^{4/3}$.

finite-size scaling ansatz

$$V(x, L) \sim L^{2/\nu}\tilde{V}((x - x_c)L^{1/\nu}), \tag{14}$$

(which is equivalent to (2) of [2]) where $\tilde{V}(y)$ is a scaling function. From this it follows that the position and the height of the peak in $V(x, L)$ scale as $x_c(L) - x_c \sim L^{-1/\nu}$ and $V_{\max}(L) \sim L^{2/\nu}$.

In table 3 we have listed the numerical values of the mean-length at x_c and the position and height of the maximum of the fluctuations. We analyse these data by forming the associated generating functions, $N(z) = \sum_L \langle n(x, L)\rangle z^L$ etc, and using differential approximants. Given the expected asymptotic behaviour of these quantities the generating functions should have a singularity at $z_c = 1$ with critical exponents $-1/\nu - 1$ (average length at x_c), $1/\nu - 1$ (position of the peak) and $-2/\nu - 1$ (height of the peak). In table 4 we list the results from an analysis of the generating functions using second-order differential approximants. The estimates for the exponents are not very accurate (which is not surprising given the short length of the series) but are fully consistent with $\nu = 3/4$.

Finally, in figure 9 we perform a more detailed analysis to confirm the conjectured scaling form for $V(x, L)$. In the top-left panel we have simply plotted $V(x, L)$ as a function of the fugacity x to confirm the single peak behaviour. In the top-right panel we have plotted $x_c(L)$ and $V_{\max}$ versus L in a log–log plot, thus confirming that these quantities grow as a power-law with L (the straight lines, drawn as a guide to the eye, have slopes $-1/\nu = -4/3$ and $2/\nu = 8/3$, respectively). In the bottom panels we check numerically

Table 3. The mean-length of walks crossing an $L \times L$ square at the critical fugacity $x = x_c$, the position, $x_c(L) - x_c$, and height, $V_{\max}(L)$, of the peak in the fluctuations $V(x, L)$.

L	$\langle n(x_c, L)\rangle$	$x_c(L) - x_c$	$V_{\max}(L)$
1	2		
2	4.123 082 7138	0.937 021 7352	2.535 898 3849
3	6.349 107 8353	0.555 468 7338	6.285 074 3202
4	8.651 936 5910	0.396 396 0508	12.567 128 9312
5	11.012 977 3423	0.301 671 4640	21.624 667 6036
6	13.418 756 1852	0.240 344 8999	33.750 732 8831
7	15.859 348 0600	0.197 967 3072	49.226 822 0069
8	18.327 354 5355	0.167 198 1710	68.329 430 9970
9	20.817 197 6528	0.143 980 1106	91.328 882 5240
10	23.324 624 3077	0.125 915 8112	118.488 718 5709
11	25.846 355 6412	0.111 509 1953	150.065 708 9122
12	28.379 836 9044	0.099 783 2765	186.310 146 0060
13	30.923 057 2826	0.090 075 3740	227.466 246 9752
14	33.474 418 7854	0.081 921 3689	273.772 578 8463
15	36.032 639 8605	0.074 987 2153	325.462 469 6518
16	38.596 683 8209	0.069 026 7737	382.764 390 1657
17	41.165 705 1788	0.063 854 9420	445.902 301 5941

Table 4. Estimates for z_c and the critical exponents obtained from second-order differential approximants to the generating functions in table 3. K is the degree of the inhomogeneous polynomial of the differential approximant.

	$\langle n(x_c, L)\rangle$		$x_c(L) - x_c$		$V_{\max}(L)$	
K	z_c	$-1/\nu - 1$	z_c	$1/\nu - 1$	z_c	$-2/\nu - 1$
0	0.999 9823(13)	−2.329 85(17)	1.000 17(11)	0.3147(96)	0.999 998(20)	−3.662 0(21)
1	0.999 983(10)	−2.329 9(12)	1.000 114(23)	0.3196(16)	0.999 9900(41)	−3.661 34(34)
2	0.999 9818(79)	−2.329 73(99)	1.000 124(15)	0.3185(16)	0.999 982(10)	−3.660 6(10)
3	0.999 9789(88)	−2.329 3(11)	1.000 13(10)	0.3183(81)	0.999 975(17)	−3.659 8(18)
4	0.999 9773(76)	−2.329 15(93)	1.000 084(45)	0.3215(47)	0.999 979(11)	−3.660 3(11)
5	0.999 9786(70)	−2.329 30(80)	1.000 136(75)	0.3171(61)	0.999 9850(69)	−3.660 81(65)

the scaling ansatz for $V(x, L)$. In the left panel we plot $V(x, L)/L^{8/3}$ versus the scaling variable $(x - x_c)L^{4/3}$ obtaining a reasonable scaling collapse. A better idea of the quality of the scaling collapse can be gauged from the plot in the bottom-right panel. Here we plot the difference between consecutive scaling plots from the left panel. More precisely, we plot $D(x, L) = V(x, L)/L^{8/3} - V(x', L - 1)/(L - 1)^{8/3}$ versus $(x - x_c)L^{4/3}$, where x' is chosen so that the scaled variables coincide, e.g., $(x - x_c)L^{4/3} = (x' - x_c)(L - 1)^{4/3}$.

8. Walks crossing the square and hitting the centre

In [12] Knuth also considered the problem of self-avoiding walks crossing the square *and* passing through the centre $(L/2, L/2)$ of the grid (with L being even). Denote the number of such walks by $c(L)$. Then a straightforward variant of the method of proof used in section 4 can be applied to prove that

$$\lim_{L\to\infty} c(L)^{1/L^2} = \lambda^2.$$

Knuth used Monte Carlo simulations to estimate the fraction of paths hitting the centre point and found for $L = 10$ that 81 ± 10 per cent of all paths do hit the centre. He then went

Table 5. The total number of walks crossing an $L \times L$ square and passing through the centre $(L/2, L/2)$, $c(L)$ and the ratio $c(L)/C(L)$.

L	$c(L)$	$c(L)/C(L)$
2	10	0.833 333 ...
4	7 056	0.828 947 ...
6	462 755 440	0.803 701 ...
8	2 593 165 016 903 538	0.793 842 ...
10	1 243 982 213 040 307 428 318 660	0.792 972 ...
12	51 166 088 445 891 978 924 432 033 203 830 714	0.792 927 ...
14	180 349 587 397 776 823 066 172 713 933 745 722 978 533 730 900	0.792 920 ...
16	54 508 896 286 415 931 462 305 055 600 895 616 388 822 171 335 171 594 099 162 334	0.792 909 ...
18	1 413 040 380 714 086 952 244 299 343 879 218 154 884 335 669 707 058 802 937 825 791 571 640 010 167 156	0.792 901 ...

on to say that ”perhaps nobody will ever know the true answer.” Naturally, we cannot let Knuth’s challenge go unanswered. It is very simple to modify the transfer matrix algorithm to ensure that all paths pass through a given vertex. We just make sure that when we do the updating at the given vertex the input state ‘00’ (no occupied incoming edges) has only one output state ‘12’, while the output ‘00’ (no outgoing occupied edges) is disallowed at this vertex. We can thus answer Knuth’s query and state for all to know that for $L = 10$ a fraction $1243\,982\,213\,040\,307\,428\,318\,660/1568\,758\,030\,464\,750\,013\,214\,100 = 0.792\,972\ldots$ of all paths pass through the centre. In table 5 we have listed the number of paths passing through the centre for $L \leqslant 18$.

The fact that $C(L)/c(L)$ appears to be going to a constant implies that not only is the asymptotically dominant behaviour of both $C(L)$ and $c(L)$ the same, but so must the sub-dominant behaviour. We note the useful mnemonic that the ratio appears close to $\sqrt{\pi/5} = 0.792\,66\ldots$, though we have no idea how to prove or disprove that this is the correct value.

9. Hamiltonian walks

Hamiltonian walks can only exist on $2L \times 2L$ lattices. For lattices with an odd number of edges, one site must be missed. A Hamiltonian walk is of length $4L(L+1)$ on a $2L \times 2L$ lattice. The number of such walks grows as τ^{4L^2}, where we find $\tau \approx 1.472$ based on exact enumeration up to 17×17 lattices. In [10] Jacobsen and Kondev gave a field-theoretical estimate of the growth constant for a Hamiltonian SAW on the square lattice as $1.472\,801 \pm 0.000\,01$. These were walks confined to a square geometry, but not restricted as to starting and endpoints as are those we consider here. Nevertheless, it seems likely that we are estimating the same quantity, so our results can be seen as providing support for the view that the field theory is estimating precisely the same quantity as our enumerations. That is to say, this appears to be precisely the same as the corresponding result for Hamiltonian walks on an $L \times L$ lattice, in the large L limit. These estimates are about 20% less than λ, the growth constant for all paths. In [1] it is proved that $2^{1/3} \leqslant \tau \leqslant 12^{1/4}$. Numerically, this evaluates to $1.260 \leqslant \tau \leqslant 1.861$.

We can improve on these bounds as follows. We define cow-patch walks to be Hamiltonian if every vertex of the square not belonging to the border of the square belongs to one of the SAWs of the cow-patch. Then the upper bounds given above translate verbatim into upper bounds for τ, while lower bounds are given by Hamiltonian traversing paths and equation (8). In this way we find that $1.429 < \tau < 1.530$. As we have shown above that $1.6284 < \lambda$, this proves that $\tau < \lambda$.

Table 6. The number of Hamiltonian paths.

L	H_L
1	2
2	2
3	32
4	104
5	10 180
6	111 712
7	67 590 888
8	2 688 307 514
9	9 628 765 945 000
10	1 445 778 936 756 068
11	29 725 924 602 729 604 016
12	17 337 631 013 706 758 184 626
13	1 998 903 003 325 610 328 086 958 408
14	4 628 650 743 368 437 273 677 525 554 148
15	2 937 440 223 891 635 053 435 045 277 805 847 436
16	27 478 778 338 807 945 303 765 092 195 103 685 118 924
17	94 555 056 448 262 478 314 997 568 263 027 383 699 860 223 148

Table 7. The number of Hamiltonian cow-patch paths.

L	HP_L
2	6
3	81
4	2 420
5	158 487
6	22 668 546
7	7 067 228 903
8	4 796 951 277 784
9	7 083 189 530 689 311
10	22 740 544 515 287 098 346
11	158 673 902 903 632 923 216 807
12	2 405 521 769 596 577 026 409 223 804
13	79 215 226 453 280 152 797 069 512 845 071
14	5 665 275 864 000 731 097 175 367 200 188 234 758
15	879 791 999 732 650 875 090 633 720 304 683 597 787 867
16	296 640 712 696 590 626 976 673 730 832 416 228 749 213 171 388
17	217 134 088 450 048 497 810 206 709 994 144 694 071 029 172 119 163 041
18	345 011 492 148 033 546 292 595 301 223 727 273 934 239 259 467 419 472 922 686

The number of Hamiltonian paths H_L for L even, and paths that visit all but one site, for L odd, are given in table 6. The number of Hamiltonian cow-patch paths HP_L for L even, and cow-patch paths that visit all but one site, for L odd, are given in table 7. The number of Hamiltonian transverse paths HT_L for L even, and transverse paths that visit all but one site, for L odd, are given in table 8.

E-mail or WWW retrieval of series

The series for the problems studied in this paper are available by request from I.Jensen@ms.unimelb.edu.au or via the world wide web http://www.ms.unimelb.edu.au/∼iwan/ by following the relevant links.

Table 8. The number of Hamiltonian traversing paths.

L	HT_L
1	2
2	8
3	34
4	650
5	12 014
6	1 016 492
7	83 761 994
8	32 647 369 000
9	12 227 920 752 840
10	22 181 389 298 814 376
11	38 166 266 554 504 010 420
12	323 646 210 116 765 453 608 746
13	2 574 827 340 090 912 815 899 810 042
14	102 299 512 403 818 451 392 332 665 527 950
15	3 778 748 215 131 699 995 997 836 850 757 543 682
16	704 314 728 645 701 361 948 084 580 318 587 261 484 806
17	121 135 616 205 759 617 794 904 559 766 506 890 558 675 949 856
18	106 005 756 542 854 454 380 006 180 528 618 254 764 945 283 647 525 384

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