SELF-AVOIDING WALKS CROSSING A SQUARE

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Abstract. We study a restricted class of self-avoiding walks (SAW) 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 give a precise estimate for λ as well as obtaining upper and lower bounds. We give exact results for the number of SAW 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 is proportional to L, while for $x>1/\mu$ it is proportional to L^2. Here μ is the growth constant of unconstrained SAW in $\mathbb{Z}^2$. For $x=1/\mu$ we provide numerical evidence, but no proof, that the average walk length is $O(L^{4/3})$.

We also consider Hamiltonian walks under the same restrictions. These 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 $\tau<\lambda$.

Nous étudions les chemins auto-évitants (CAE) du réseau carré qui partent de l'origine $(0,0)$, finissent en (L,L), et sont entièrement contenus dans le carré $[0,L]\times[0,L]$. On sait que le nombre de tels chemins croît comme $\lambda^{L^2+o(L^2)}$. Nous donnons une estimation précise, ainsi que des bornes supérieures et inférieures pour λ. Nous donnons le nombre exact de CAE de longueur $2L+2K$ traversant le carré de côté L, pour $K=0,1,2$, et le comportement asymptotique de ce nombre pour $K=o(L^{1/3})$.

On associe ensuite un poids x à chaque pas d'un chemin, ce qui mène à une modèle présentant une transition de phase. Si μ désigne la constante de croissante des CAE non contraints, alors pour $x<1/\mu$, la longueur moyenne d'un CAE traversant le carré de côté L est proportionnelle à L, tandis qu'elle est proportionnelle à L^2 lorsque $x>\mu$. Pour $x=\mu$, nos données numériques suggèrent que la longueur moyenne est en $O(n^{3/4})$.

Nous considérons aussi des chemins hamiltoniens traversant un carré. Le nombre de tels chemins croît comme $\tau^{L^2+o(L^2)}$. Nous donnons une estimation précise et des bornes supérieures et inférieures pour τ, et nous prouvons que $\tau<\lambda$.

1. Introduction

We are considering the problem of self-avoiding walks on the square lattice $\mathbb{Z}^2$. For walks on an infinite lattice, it is generally accepted [9] that the number c_n of such walks of length n, considered up to a translation, grows as $c_n \sim const.\mu^n n^{\gamma-1}$, with metric properties, such as mean-square radius of gyration or mean-square end-to-end distance growing as $\langle R^2\rangle_n \sim const.n^{2\nu}$, 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 $C(x):=\sum_n c_n x^n$, and it will be useful to define a second generating function for those SAW 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 [9] to be the rate of decay of G along a

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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 SAW 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 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 mentioned by Knuth [7], within the framework of a discussion on how to estimate large numbers. The first full discussion as a mathematical problem seems to be by Abbott and Hanson [1] in 1978, many of whose results and methods are still useful today. In [10] there is mention of a version of the problem being due to earlier work of Hammersley. A key question considered in [1] and in this paper, is the number of distinct SAW 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 SAW 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 [13] it was proved that $C_L(1)=\lambda^{L^2+o(L^2)}$. The value of λ is not known, though bounds and estimates have been given in [1, 13]. One of our purposes in this paper is to improve on both the bounds and the estimate.

In the statistical mechanics literature, the problem appears to have been introduced by Whittington and Guttmann [13] in 1990, who were particularly interested in the phase transition that takes place as one varies the fugacity 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 being proportional to L to being proportional to L^2. In [13] the critical fugacity proved to be $\geq 1/\mu$, and conjectured to be $x_c = 1/\mu$. In [8] the conjecture was proved.

In [1] the more general problem of SAW constrained to an $L\times M$ lattice was considered, where the analogous question was asked: how many self-avoiding 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 fixed, the paths can be generated by a finite dimensional transfer matrix, and hence that the generating function is rational. Indeed, in [1] it was proved that

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

(where here we have corrected a typographical error). It follows that $C_{L,2} \sim \text{const.}\lambda_2^{2L}$, where $\lambda_2 = \sqrt{\frac{2}{\sqrt{13}-3}} = 1.81735\ldots$.

In this paper we also consider two further problems which can be seen as generalisations of the stated problem. Firstly, we consider the problem where SAWs are allowed to start anywhere on the left edge of the square and terminate anywhere on the right edge; so these are walks *spanning* the rectangle from left to right. We denote by T_L the number of such SAWs on an $L\times L$ lattice. Secondly, we consider the problem in which there may be several independent self- and mutually-avoiding walks, each such walk starting and ending on the perimeter of the square. The SAW are not allowed to take steps along the edges of the perimeter. Such walks partition the rectangle into distinct regions and by colouring the regions alternately black and white we get a *cow-patch* pattern. We denote by P_L the number of such configurations of SAWs on an $L\times L$ lattice. Each problem is illustrated in figure 1. These generalisations are introduced as they allow us to establish rigorous bounds on λ, which we do below.

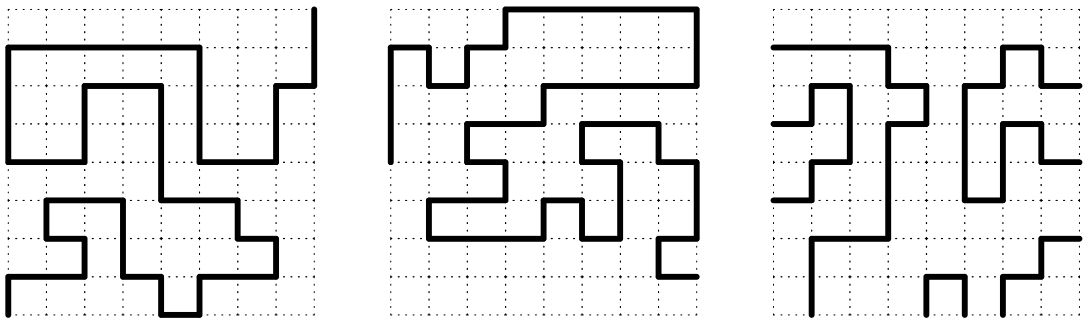

FIGURE 1. An example of a SAW configuration crossing a square (left panel), spanning a square from left to right (middle panel) and a cow-patch (right panel).

Following the work in [13], Madras in [8] proved a number of theorems. In fact, most of Madras's results were proved for the more general d-dimensional hypercubic lattice, but here we will quote them in the more restricted two-dimensional setting.

Theorem 1. *The following limits,*

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

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

More precisely,

(*i*) $\mu_1(x)$ *is finite for* $0 < x \leq 1/\mu$, *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* $0 < x \leq 1/\mu$ *and* $\mu_2(x) > 1$ *for* $x > 1/\mu$.

The average length of (weighted) walks crossing the $L \times L$ square is defined to be

$$\langle n(x)\rangle_L := \sum_n n c_n(L) x^n / \sum_n c_n(L) x^n. \tag{3}$$

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,

$$\kappa_1\, b(x) \leq a(x) \leq \kappa_2\, b(x).$$

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

The situation at $x = 1/\mu$ is unknown. We provide compelling numerical evidence that in fact $\langle n(1/\mu)\rangle_L = \Theta(L^{1/\nu})$, where $\nu = 3/4$, in accordance with an intuitive suggestion in [8].

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* $0 < f_2(x) \leq \log \mu + \log x$.

Some, but not all of the above results were previously proved in [13], but these three theorems elegantly capture all that is rigorously known.

2. 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 [13].

2.1. 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 essentially 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 $C_{L,L} \leq 2^{L^2}$. Of the 16 possible 2×2 matrices, only 14 can correspond to portions of non-intersecting lattice paths. Lote 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 $C_{L,L} \leq 14^{(L/2)^2}$, so $\lambda \leq 1.9343...$ Similarly, for 3×3 lattices we find 320 admissible matrices (out of a possible 512), so $\lambda \leq 320^{1/9} = 1.8982..$ For 4×4 lattices, [1] claims that there are 22662 admissible matrices, but we believe the correct number to be 22816, giving the bound $\lambda \leq 1.8723...$ 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 3.5465202×10^{90} such matrices, giving the bound

$$\lambda \leq 1.781684.$$

This bound is fully equivalent to the bound $\lambda \leq (2P_L)^{1/L^2}$, where P_L denotes the number of cow-patch configurations on the $L \times L$ lattice. This equivalence follows if one colours 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.

2.2. Lower bounds on λ

In [1] the useful bound

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

is proved.

The above evaluation of λ_2, see (2), 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 $M \leq 6$. 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: $\lambda_3 = 1.76331\ldots$, $\lambda_4 = 1.75146\ldots$, $\lambda_5 = 1.74875\ldots$ and $\lambda_6 = 1.74728\ldots$ from which we obtain the bound $\lambda > 1.61339\ldots$.

However, an alternative lower bound can be obtained from spanning SAWs, defined in Section 1. If T_L denotes the number of spanning SAW on the $L \times L$ lattice, then we prove in the full version of this paper that

$$\lambda \geq T(L)^{1/((L+1)(L+2))}. \tag{4}$$

This gives the improved bound $\lambda > 1.6284$.

Combining our results for lower and upper bounds finally gives

$$1.6284 < \lambda < 1.781684.$$

3. Computer 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 spanning a square and the cow-patch configurations.

3.1. The algorithm

The basic algorithm used to enumerate self-avoiding walks crossing a square is based on the method of Conway et al. [2] for enumerating ordinary self-avoiding walks. The number of walks crossing an $L \times M$ rectangle is counted using a transfer matrix algorithm. The transfer matrix technique involves drawing a boundary line through the rectangle intersecting

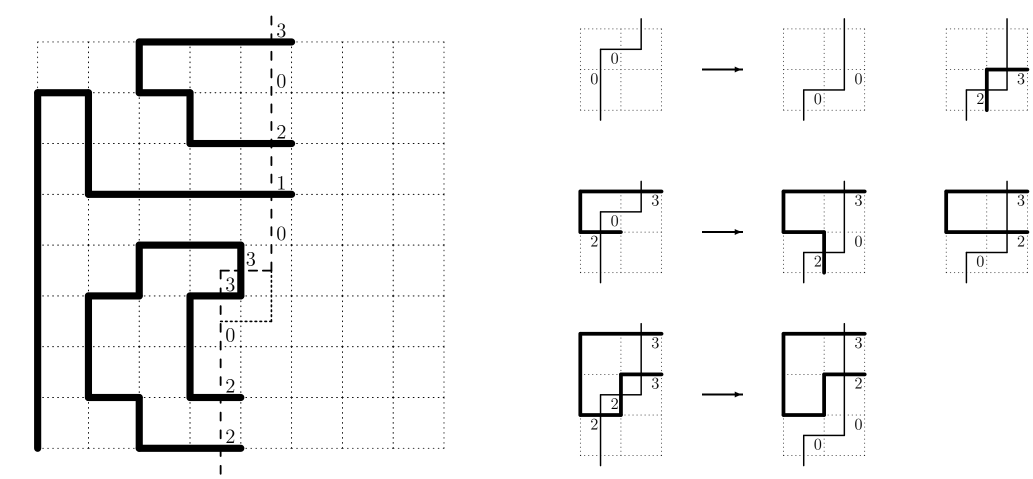

Figure 2. The left panel shows a snapshot of the intersection (dashed line) during the transfer matrix calculation. Walks within a rectangle are enumerated by successive moves of the kink in the boundary, as exemplified by the position given by the dotted line, so that the $L \times M$ rectangle is built 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.

up to $M + 2$ 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 must indicate if the ith edge of the boundary is occupied or empty. An empty edge is indicated by $\sigma_i = 0$. An occupied edge is either *free* (that is, not connected to other edges of the boundary by a path located to the left of the boundary) or connected to exactly one such edge. 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 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 2's equals the total number of 3's. Furthermore, as we look through the configuration from the bottom the number of 2's is never smaller than the number of 3's (so that configurations can be seen as well-balanced parentheses systems). 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.

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.

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

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 are 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 (below) the horizontal part of the boundary. Some of the update rules are illustrated further in figure 2. The topmost 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 represents 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 bottommost panels represents 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 relabeling of the matching loop-end when connecting two '2's (or two '3's) is denoted by over-lining 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 relabeling 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. 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.

3.2. Complexity

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, $N_{\text{conf}}(M)$, exactly. Obviously the free end cuts the boundary line configuration into two separate pieces. Each of these pieces consists of '0's and an equal number of '2's and '3's with the latter forming a well-balanced parenthesis system.

Each piece thus corresponds to a *Motzkin path* [12, Ch. 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

$$\mathcal{M}(x) = [1 - x - ((1+x)(1-3x))^{1/2}]/2x^2. \tag{5}$$

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

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

When the boundary line has a kink the number of configurations exceeds $N_{\text{conf}}(M)$ but clearly is less than $N_{\text{conf}}(M+1)$. From (5) we see that asymptotically $N_{\text{conf}}(M)$ 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 a walks grows like λ^{LM} and our algorithm thus 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 [6]. 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 $p_1 p_2 \cdots p_k > m$.

3.3. Extensions of the algorithm

The algorithm is easily generalised 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 generalisation to study walks crossing a square, the generating function is a polynomial of degree (at most) M^2 in x. The coefficient of x^n in this polynomial is the number of walks of length n intersecting the boundary line in the pattern specified by the configuration. When the boundary is updated, if m additional steps are inserted, the generating function of the source is multiplied by x^m and added to the generating function of the target. Not all M^2 terms in the polynomials need be retained. Firstly, only terms with n even are non-zero and only these are retained. Secondly, in order to construct a given boundary line configuration, a certain minimal number of steps $n_{\min}$ are required and terms with $n < n_{\min}$ can be discarded.

The generalisation to spanning walks is also quite simple. Firstly, we have $M+1$ initial configurations which are empty except for a free end at position $0 \leq j \leq M$. 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 spanning an $L \times M$ rectangle.

The generalisation to cow-patch patterns is more complicated. Graphs can now have many separate components and there can be many free ends in a boundary line configuration. Note also that each free end has to start and terminate with a step perpendicular to the border of the rectangle and there are no 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. 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 is 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 relabeling 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.

3.4. Results

As discussed above, in order to obtain the exact value of the number of SAW 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 hours using 8 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 $L \leq 17$. In other words, we have obtained the polynomials $C_L(x)$ for $L \leq 17$. In addition, we have computed $C_{18}(1)$ and $C_{19}(1)$, the total number of SAW crossing an 18×18 and 19×19 square respectively. We have also computed the corresponding quantities for cow-patch and spanning SAWs, denoted $P_L(1)$ and $T_L(1)$ respectively, for $L \leq 19$.

Finally, 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. Numerical analysis

It has been proved [1, 13] that $\lim_{L\to\infty} C_{L,L}^{\frac{1}{L^2}} = \lambda$ exists. From this it is reasonable to expect (but not a logical consequence) that $R_L = C_{L+1,L+1}/C_{L,L} \sim \lambda^{2L}$ so the generating function $\mathcal{R}(x) = \sum_L R_L x^L$ has a radius of convergence $x_c = 1/\lambda^2$, which we can estimate accurately using differential approximants [4]. We estimate in this way that for the crossing problem $x_c = 0.32858(5)$, for the spanning problem $x_c = 0.3282(6)$ and for the cow-patch problem $x_c = 0.328574(2)$. So we see that λ is the same for the three problems, and we estimate that $\lambda = 1.744550(5)$. It is not difficult to prove that λ defined for SAW crossing a square, and for spanning walks takes the same value. For cow-patch walks, this is somewhat more difficult, but we have done so (see the full version of this paper).

We now speculate on the sub-dominant terms. For SAW on an infinite lattice, it is widely accepted (but not proved) that $c_n \sim const.\mu^n n^g$, where c_n is the number of n step SAW equivalent up to a translation.

It seems reasonable to speculate that, the number of SAWs crossing an $L \times L$ lattice is equivalent to $A\lambda^{L^2+bL}L^\alpha$. We have investigated this possibility numerically, and found it to be well supported by the data.

For cow-patches we find $b \approx 0.8558$ and $\alpha \approx -0.500$. For transverse walks and walks crossing a square b is quite small, possibly zero. For transverse walks we find $\alpha \approx 1.75$ while for walks crossing the square $\alpha \approx 0$. This suggests asymptotic behaviours $A_P\lambda^{L^2+0.8558L}/\sqrt{L}$, $A_T\lambda^{L^2}L^{7/4}$ and $A_W\lambda^{L^2}\log L$ respectively, where A_P, A_T, and A_W can be estimated, and the $\log L$ term (or some power of a logartihm) would follow if α were exactly zero.

As remarked in the introduction, we have also studied (numerically) the behaviour of $\langle n(1/\mu)\rangle_L$, by a log-log plot as well as other numerical methods. The results are totally consistent with the conjecture [8], that $\langle n(1/\mu)\rangle_L$ is proportional to $L^{1/\nu}$, where $\nu = 3/4$.

5. Asymptotics for walks of "small" length crossing a square

We now consider walks of length $2L + 2K$ crossing an $L \times L$ square. Note that walks of length $2L$ are the minimal possible length. With $K = 0$ the number of possible walks is $\binom{2L}{L}$. This result is obvious, as there are $2L$ steps in the path, of which L must be in the positive x (and of course positive y) direction. Note that this has the asymptotic expansion

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

With $K = 1$ we have proved that the number of possible paths is given by $2L\binom{2L}{L+2}$. This result has the asymptotic expansion

$$2L\binom{2L}{L+2} = \frac{L4^L}{\sqrt{L\pi}}\left(2 - \frac{33}{4L} + \frac{1345}{64L^2} - \frac{23835}{512L^3} + \mathrm{O}\left(L^{-4}\right)\right).$$

For $K = 2$ we have proved that the number of possible paths is given by

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

This has asymptotic expansion

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

Our technique can be, in theory, extended to count walks of length $2L + 2K$, for any given value of K. It proves that the sequence of numbers thus obtained is always *P-recursive*. That is to say, it satisfies a linear recurrence relation with polynomial coefficients [11]. But, even for $K = 3$, the number of special cases that must be treated becomes very large. We have resorted to a numerical study for higher values of K, and for $K = 3$ we found

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

while the corresponding result for $K = 4$ is

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

We can give an heuristic argument for the general form of the leading term in the asymptotic expansion of the case $K = k$, which leads to the leading order term $\frac{4^L}{\sqrt{L\pi}} \frac{(2L)^k}{k!}$. Here the first term 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 [3].

6. Hamiltonian walks crossing a square

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. This is about 20% less than λ, the growth constant for all SAWs. In [5] the estimate of the growth constant for Hamiltonian SAW on the unconstrained square lattice 1.472801 ± 0.00001 was given. This should be precisely the same as the corresponding result for Hamiltonian walks on an $L \times L$ lattice, in the large L limit. In [1] it is proved that $2^{1/3} \leq \tau \leq 12^{1/4}$, that is to say, $1.260 \leq \tau \leq 1.861$. We can improve on these bounds as follows: we define generalized 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 spanning walks and (4). In this way we find $1.429 \leq \tau \leq 1.52999$. As we have shown above that $1.6284 < \lambda$, this proves that $\tau < \lambda$.

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