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Self-avoiding walks of specified lengths on rectangular grid graphs

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Abstract. The investigation of self-avoiding walks on graphs has an extensive literature. We study the notion of wrong steps of self-avoiding walks on rectangular shape $n \times m$ grids of square cells (Manhattan graphs) and examine some general and special cases. We determine the number of self-avoiding walks with one and with two wrong steps in general. We also establish some properties, like unimodality and sum of the rows of the Pascal-like triangles corresponding to the walks. We also present particular recurrence relations on the number of self-avoiding walks on the $n \times 2$ grids with any specified number of wrong steps.

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1. Introduction

A self-avoiding walk on a graph is a walk that never visits the same vertex more than once. In the literature, self-avoiding walks have been extensively studied on both finite and infinite graphs. A central problem in this area, motivated by the study of polymer chains, is to consider the number of distinct self-avoiding walks of a prescribed length starting at the origin on the integer lattice $\mathbb{Z}^d$ (for a general overview of the topic, see the book of Madras and Slade [17]). Although this original problem seems to be very intractable in general, and even its asymptotic behaviour holds open questions, the problem of self-avoiding walks can be dealt with under certain restrictions or by considering them on different graphs. Some examples of infinite graphs on which self-avoiding walks have been investigated are lattice strips $\{0, \dots, m\} \times \mathbb{Z}$ with finite m [5,9,24,25], the hexagonal lattice [11] or hyperbolic graphs [3,18]. For finite domains, examples are square grids [4,6,8,13,14,16,23], rectangular grids [1,12,19,20], or complete graphs [10,21].

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We limit our investigation of self-avoiding walks to rectangular grid graphs. In the case of square or rectangular grid graphs, the original question asks for the total number of self-avoiding walks starting from one corner vertex and ending at the opposite corner vertex (i.e., the length of the walks is not restricted to a predefined value) and confined to lie entirely within its domain (including its boundaries). Recently, there has also been increased interest in constructions where either the starting and ending vertices are not necessarily at the corners of the domain [6,7,14,19,20], or some constraint is placed on the direction of the steps [4,12]. We follow the classical approach in the sense that we consider self-avoiding walks between vertices at opposite corners, but with restrictions on the length of the walks and the direction of the steps. Using elementary combinatorial techniques, we give closed-form formulas and recursive relations for the cardinality of certain sets of self-avoiding walks.

First, we fix the terminology used in the present work to avoid misconceptions. The vertex (or grid point) set of an $n \times m$ *rectangular grid graph* (or $n \times m$ *grid* for short) is given by the Cartesian product $\{0, 1, \ldots, n\} \times \{0, 1, \ldots, m\}$ for some $n, m \in \mathbb{N}$, and any two of its vertices (a, b) and (c, d) are adjacent if $|a - c| + |b - d| = 1$. In this paper, we mostly figure such a graph in the planar Cartesian system, where the vertices have coordinates (a, b) with $0 \leq a \leq n$ and $0 \leq b \leq m$. But sometimes we illustrate the graph identically to the structure of Pascal's triangle. We investigate the number of distinct self-avoiding walks on the $n \times m$ grid starting at the vertex $(0, 0)$ and ending at the vertex (n, m). A self-avoiding walk is sometimes called path.

We say that the edge $\{(a, b), (c, d)\}$ of a walk on a rectangular grid is an *east* (*west, north, south*) *step* if (a, b) precedes (c, d) in the vertex sequence of the walk and $a - c = -1$ ($a - c = 1$, $b - d = -1$, $b - d = 1$, respectively). The expression *right* (*left*, *up*, *down*, respectively) *step* is also used as a synonym. We say that an edge of a walk is a *wrong step* (or *error step*) if it is a south step or a west step. Obviously, a shortest path between $(0, 0)$ and (n, m) on the $n \times m$ grid does not include wrong steps. Let $T^{(w)}(n, m)$ denote the number of distinct self-avoiding walks from $(0, 0)$ to (n, m) on the $n \times m$ grid that contain exactly $w \in \mathbb{N}$ wrong steps. Figure 1 illustrates three self-avoiding walks on the 6×4 grid. Here and throughout the paper, a wrong step is highlighted by a red arrows.

The cells of the grid constitute an $n \times m$ *board*, and sometimes we refer to a cell of the grid by using its location in a column or row of the board. Moreover, the aggregation of two edge-neighbour cells is called *domino*.

Pascal's triangle can be interpreted as the bivariate function defined on $\mathbb{N}^2$ whose value at the point (n, m) is the number of the shortest walks on the $n \times m$ grid between the vertices $(0, 0)$ and (n, m). The shortest walks are, of course, free of error steps (i.e., $w = 0$), and consist of exactly $(n + m)$ steps, n east steps and m north ones. Hence, using our notation

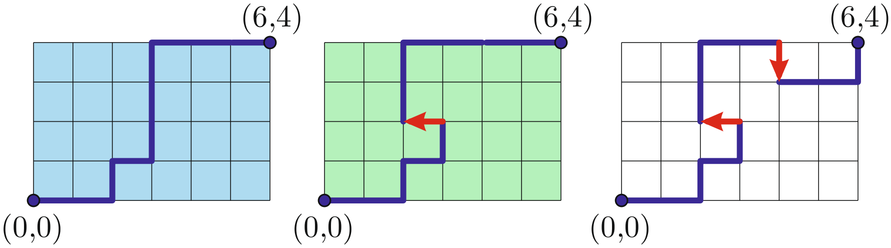

FIGURE 1. Walks with 0, with 1, and with 2 wrong steps on the 6×4 grid

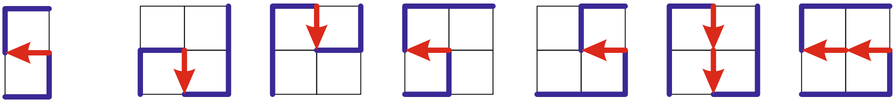

FIGURE 2. Walks with wrong steps on 1×2 and 2×2 grids

$$T^{(0)}(n,m) = \binom{n+m}{n}. \tag{1}$$

The triangular arrangement $\mathcal{T}^{(0)}$ of the binomial coefficient (i.e., Pascal's triangle, where $T^{(0)}(n,m)$ appears in the nth entry of row $(n+m)$) allows us to extend this concept to arbitrary $w \in \mathbb{N}$ as we introduce a new family of generalized Pascal's triangles. For $w \in \mathbb{N}$, we define the triangular array $\mathcal{T}^{(w)}$ by setting $(n,m) \mapsto T^{(w)}(n,m)$, which admits the number of self-avoiding walks on the $n \times m$ grid containing exactly w wrong steps. Triangles $\mathcal{T}^{(1)}$ and $\mathcal{T}^{(2)}$ are illustrated in Sects. 2 and 3, respectively. The sum $\sum_{n=0}^{\nu} T^{(w)}(n, \nu - n)$ of the terms in the row ν of $\mathcal{T}^{(w)}$ gives the number of all self-avoiding walks with w wrong steps to the points which have distance ν from the origin.

Furthermore, Figs. 2 and 3 illustrate all the walks with wrong steps on the 1×2, 2×2, and 3×2 grids.

The exact enumeration of the self-avoiding walks on a rectangular grid becomes more and more burdensome as the number w increases. For this reason, we will confine ourselves to examining only the cases $w = 1$ and $w = 2$ in general. The principal results are explicit formulas for $T^{(1)}(n,m)$ and $T^{(2)}(n,m)$ established in Sects. 2 and 3, respectively. These generalize the results of Bousquet-Mélou, Guttmann, and Jensen in [6, Sec. 6] to rectangular grids. We also examine the rows and diagonals in the triangle $\mathcal{T}^{(1)}$. In addition, we will investigate $n \times m$ grids for arbitrary w with the restriction $m \leq 2$ in Sect. 4. The case $n \times 1$ is quite easy, while the $n \times 2$ grid requires a more complicated description.

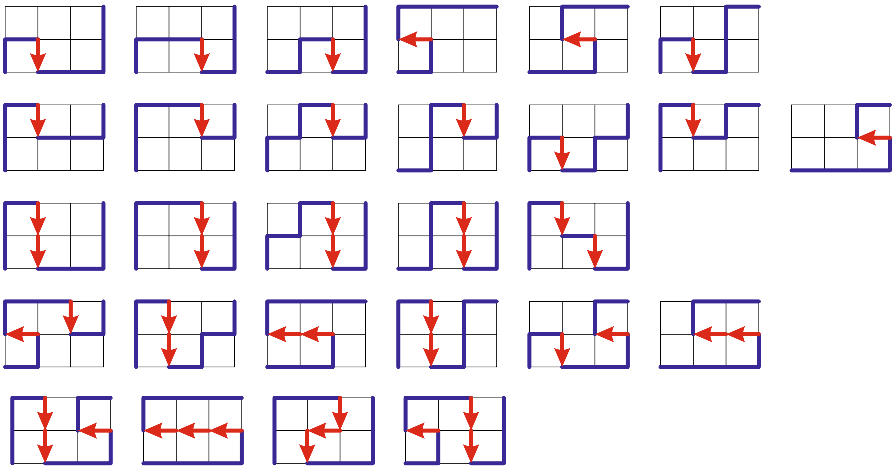

FIGURE 3. Walks with wrong steps on the 3×2 grid

At the end of this section, we quote a lemma, and a very powerful theorem, which will be useful in the proofs later. The lemma is a known result, one can find it, for instance, in the famous book of Knuth [15, p. 59, (25)]. As usual for non-negative a the binomial coefficient $\binom{a}{c}$ vanishes if the integer c is negative or larger than a.

Lemma 1. *Let a, b, c, d be non-negative integers, $d \geq b$. Then*

$$\sum_{k=0}^{a} \binom{a-k}{c} \binom{b+k}{d} = \binom{a+b+1}{c+d+1}.$$

The next general result is Theorem 3.1 in [2] of Ahmia and Szalay. It gives a widely applicable description for the weighted diagonal sums in Pascal's triangle, where the weight sequence is an arbitrary homogenous linear recurrence. Assume that a linear recursive sequence of order $s \geq 1$ is given by $G_0, \ldots, G_{s-1}$, and $G_n = \sum_{j=1}^{s} A_j G_{n-j}$, where the real coefficients $A_1, \ldots, A_s$ are fixed. Further let x and y denote two non-zero real numbers. Suppose that the integers r, q and p satisfy the conditions $r \in \mathbb{N}^+$, $q \in \mathbb{Z}$, $r + q > 0$ and $0 \leq p < r$. Put $\omega = \lfloor (n-p)/(q+r) \rfloor$.

Theorem 1. *The terms*

$$H_n = \sum_{k=0}^{\omega} \binom{n-qk}{p+rk} x^{n-p-(r+q)k} y^{p+rk} G_k$$

								0								
							0		0							
						0		0		0						
					0		1		1		0					
				0		4		4		4		0				
			0		10		13		13		10		0			
		0		20		34		36		34		20		0		
	0		35		75		91		91		75		35		0	
0		56		146		208		224		208		146		56		0

FIGURE 4. Triangle $\mathcal{T}^{(1)}$

satisfy the recurrence relation

$$H_n = xH_{n-1} - \sum_{j=1}^{rs-1} (-1)^j \binom{rs-1}{j} x^j (H_{n-j} - xH_{n-j-1}) + \sum_{t=1}^{s} A_t y^{rt} \sum_{j=0}^{r(s-t)} (-1)^j \binom{r(s-t)}{j} x^j H_{n-(r+q)t-j}$$

for all $n \geq \max\{rs, (r+q)s\}$.

2. Walks with one wrong step on the $n \times m$ grid

The main result of this section (Theorem 2) gives an explicit formula for $T^{(1)}(n,m)$. Then we find the sum of the terms of rows in the triangle $\mathcal{T}^{(1)}$ (Lemma 2) which shows the number of self-avoiding walks with a given distance with one error step. We also prove the unimodality of the terms of each sum (Theorem 4). Finally, we reveal the factorization properties of the polynomials belonging to the diagonal sequences in $\mathcal{T}^{(1)}$ (Theorems 5 and 6).

Figure 4 shows the non-negative integers $T^{(1)}(n,m)$ in triangular arrangement $\mathcal{T}^{(1)}$, where $T^{(1)}(n,m)$ appears in the nth entry of row $(n+m)$.

2.1. Explicit formula for $T^{(1)}(n,m)$

Theorem 2. *The number of self-avoiding walks with $w = 1$ wrong step on an $n \times m$ grid is*

$$T^{(1)}(n,m) = n\binom{n+m}{n+2} + m\binom{n+m}{m+2}. \tag{2}$$

The proof ascertains that the first term of the sum (2) gives the number of walks with a horizontal (west) error step, while the second term concerns the number of walks with a vertical (south) wrong step.

Proof. $T^{(1)}(n,0) = T^{(1)}(0,m) = 0$ trivially holds, as well as $T^{(1)}(1,1) = 0$. It is easy to see that for $n \geq 2$ we have $T^{(1)}(n,1) = \binom{n+1}{3}$. Indeed, there exist $n+1$ vertical edges in the grid, and we must choose 3 of them, the first to step up, the second to come down, and the third to step up again. Similarly, based on the symmetry $T^{(1)}(1,m) = \binom{m+1}{3}$.

In the sequel, we assume that $n \geq 2$ and $m \geq 2$. We will show that there exist

$$n\binom{n+m}{n+2} \tag{3}$$

self-avoiding walks with a west wrong step, and then the symmetry implies the statement of the theorem. The crucial point is to prove that there exists a bijection between the walks with one west error step on an $n \times m$ grid and the *inner* horizontal steps of the error-free walks on an $(n+2) \times (m-2)$ grid. A horizontal step is called inner if it is neither in the 1st nor in the nth column of the square cells generated by the grid. Since the number of the error-free walks is

$$\binom{(n+2)+(m-2)}{n+2} = \binom{n+m}{n+2},$$

each has n inner steps, then (3) follows.

Consider an error-free walk on an $(n+2) \times (m-2)$ grid, and take an arbitrary inner horizontal step S_i of it. S_i splits the walk into two parts, which are denoted by $\mathcal{P}_1$ and $\mathcal{P}_2$ (see Fig. 5). Replace S_i by the domino  such that $\mathcal{P}_2$ now connects to the upper right corner of the domino on an $(n+2) \times m$ grid. Then reflect the domino around its left vertical skirt so that $\mathcal{P}_2$ joins to the upper left corner of the reflected domino.

This operation ensures the only wrong horizontal step on the resulting $n \times m$ grid, and $\mathcal{P}_1$ and $\mathcal{P}_2$ appear in the new walk in the two sides of the error domino. It is clear that the starting horizontal step must be inner, otherwise the procedure fails. Finally, we need to show that distinct error-free walks with distinct inner horizontal steps lead to distinct walks with one error step. But this is clear since the location of S_i determines the location of the error step, and if S_i is common in two error-free walks, then they differ in either $\mathcal{P}_1$ or $\mathcal{P}_2$. □

Remark 1. Besides the bijection, the combinatorial proof above is based on the known formula for the number of usual walks between two points of a grid. It allows us a second proof of the theorem which will be shortly sketched here. Calculate again the number of walks with one horizontal error step on an $n \times m$

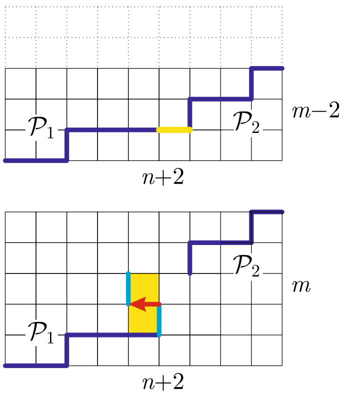

FIGURE 5. A specific transformation to produce one west wrong step

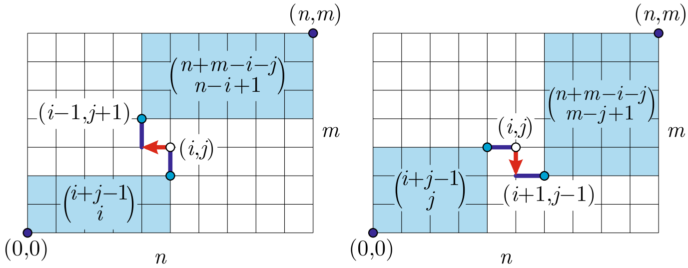

FIGURE 6. Number of walks with binomial coefficients

grid. The west error step is given by $(i, j) \longrightarrow (i-1, j)$, where $1 \le i \le n$ and $1 \le j \le m-1$ (see Fig. 6). Fixing (i, j) we compute the number of error-free walks from $(0, 0)$ to $(i, j-1)$, and also from $(i-1, j+1)$ to (n, m). Hence the sum

$$\sum_{i=1}^{n}\sum_{j=1}^{m-1}\binom{i+(j-1)}{i}\binom{(n-(i-1))+(m-(j+1))}{n-(i-1)}$$

returns with the number of walks with one horizontal wrong step. This formula, applying Lemma 1 simplifies to $n\binom{n+m}{n+2}$.

Corollary 1. *We have the recursive formula*

$$T^{(1)}(n,m) = T^{(1)}(n-1,m) + \binom{n+m-1}{n+1} + T^{(1)}(n,m-1) + \binom{n+m-1}{m+1}, \qquad n \ge 1, m \ge 1. \tag{4}$$

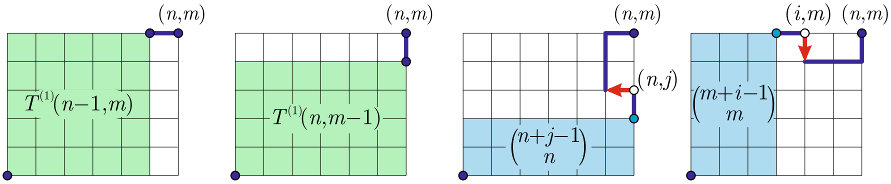

Figure 7. Explanation to the second proof of Corollary 1

Proof. The application of Theorem 2 shows immediately the statement.

An other way to prove the corollary is given by Fig. 7 which explains the roles of the terms on the right hand side of (4). Assume that the last step in the walks is $(n-1,m) \longrightarrow (n,m)$. The one error step must happen before: either we never left the $(n-1)\times m$ grid and we are now in $(n-1,m)$, or we arrived at $(n,j-1)$ without error for some $j \in \{1,\ldots,m-1\}$, and then we had one north step, then one wrong west step, which was followed by further north steps till $(n-1,m)$. The number of different ways appears as $T^{(1)}(n-1,m)$ and as $\binom{n+m-1}{n+1}$ in (4), respectively. In the latter case, the binomial coefficient resulted from the sum $\sum_{j=1}^{m-1}\binom{n+j-1}{n}$. If the last step is $(n,m-1) \longrightarrow (n,m)$, then the other two terms are obtained in (4). □

2.2. Self-avoiding walks with fixed distance ν, and sum of rows in triangle $\mathcal{T}^{(1)}$

Let ν be a non-negative integer. In this subsection, we find the number of self-avoiding walks S_ν with one wrong step to those vertices which are ν far from the origin $(0,0)$.

Clearly, $s_\nu := \sum_{n=0}^{\nu} T^{(1)}(n,\nu-n)$ provides the sum of terms when we go along the νth row of triangle $\mathcal{T}^{(1)}$ illustrated in Fig. 4. But besides s_ν there is an other component of S_ν. Indeed, $T^{(1)}(n,m)$ gives the number of ways when we never leave the rectangle with diagonal from $(0,0)$ to (n,m). In order to find S_ν we even need to consider those cases when a west wrong step happens in a point with second coordinate $m+1$, and after that we always go up vertically to reach (n,m). (Analogously, with a south wrong step, too.)

First we determine an explicit formula for the terms of $(s_\nu)_{\nu=0}^{\infty}$. For the sake of brevity we apply an "ace" theorem (Theorem 1).

Lemma 2. *For non-negative integers ν the equality*

$$s_\nu = \sum_{n=0}^{\nu} T^{(1)}(n,\nu-n) = (\nu-4)2^\nu + 2(\nu+2)$$

holds.

Proof. It is known that the sequence $G_n = n$ (for $n \in \mathbb{Z}$) satisfies the binary recurrence relation $G_n = 2G_{n-1} - G_{n-2}$. Put $k = n + 2$. Thus, together with $G_{-2} = -2$ and $G_{-1} = -1$ we have

$$\sum_{n=0}^{\nu} n\binom{\nu}{n+2} = \sum_{k=0}^{\nu}\binom{\nu}{k}G_{k-2} - (-\nu-2) = \sum_{k=0}^{\nu}\binom{\nu}{k}G_{k-2} + (\nu+2).$$

Now apply Theorem 1 for the sum $H_\nu = \sum_{k=0}^{\nu}\binom{\nu}{k}G_{k-2}$. It yields that H_ν satisfies the recursion $H_\nu = 4H_{\nu-1} - 4H_{\nu-2}$ with initial values $H_0 = -2$ and $H_1 = -3$. The characteristic polynomial $x^2 - 4x + 4 = (x-2)^2$ of the sequence H_ν, together with the initial values provide $H_\nu = (\nu/2 - 2)\,2^\nu$. Thus

$$\sum_{n=0}^{\nu} n\binom{\nu}{n+2} = \left(\frac{1}{2}\nu - 2\right)2^\nu + \nu + 2.$$

This sum is derived from the first term of (2). Because of the symmetry we double it to get the formula of the statement. □

Now we turn our attention to those cases when a west wrong step is followed by only north steps providing a unique completion of the walk. Recall that we need a north step previous to doing such a wrong step, and this north step can have starting position in the grid points of a triangle determined by the points $(1,0)$, $(\nu-2,0)$, and $(1,\nu-3)$. Since the number of ways to reach these vertices (without an error step) is given by the sum of the corresponding binomial coefficients, totally we obtain

$$\sum_{n=1}^{\nu-2}\sum_{k=0}^{\nu-2-n}\binom{n+k}{k} = \sum_{j=1}^{\nu-2}(2^j - 1) = 2^{\nu-1} - \nu.$$

In the first equality, we used the row sums of Pascal's triangle. Hence there exist $2^\nu - 2\nu$ exceptional walks with either a west or a south wrong step. We present the sum $S_\nu = s_\nu + (2^\nu - 2\nu)$ resulting from the last argument and Lemma 2 in the following

Theorem 3. *The number of self-avoiding walks to distance ν is*

$$S_\nu = (\nu-3)2^\nu + 4, \qquad (\nu \geq 1).$$

Proof. The proof is given above, but here we even provide a nice and short combinatorial proof as well. Assume that the north step before the wrong west step happens in the jth step ($j = 2, \ldots, \nu-1$) of the self-avoiding walk. For the previous $j-1$ steps we have $2^{j-1} - 1$ possibilities in total since we exclude the only north steps before. After the wrong west step we step north, and then we have exactly $2^{\nu-j}$ ways to finish the walk. That is

$$\sum_{j=2}^{\nu-1}(2^{j-1} - 1)2^{\nu-j} = (\nu-2)2^{\nu-1} - (2^{\nu-1} - 2) = (\nu-3)2^{\nu-1} + 2$$

is the number of possibilities to go ν far with one wrong west step. Hence its double $S_\nu = (\nu - 3)2^\nu + 4$ yields the statement of the theorem. □

Remark 2. We showed Theorem 3 in two different ways. The second proof is more elegant (and combinatorial), while the first one is more informative since it presents the row sums s_ν in $\mathcal{T}^{(1)}$, too. We note that S_ν is the sequence A291526 in OEIS [22], its description there contains no details connected to self-avoiding walks.

2.3. Unimodality of rows in the triangle $\mathcal{T}^{(1)}$

The unimodality of a finite sequence is a specific feature, which often gives important information on the behavior of the sequence. Since any finite ray crossing Pascal's triangle is unimodal it is natural to examine this question for the extensions of Pascal's triangle. Here we prove only the unimodality of the rows of $\mathcal{T}^{(1)}$ (illustrated in Fig. 4).

A finite sequence $(a_0, a_1, \ldots, a_\nu)$ is called *unimodal* if there exists some index $0 \le j \le \nu$ for which

$$a_0 \le a_1 \le \cdots \le a_j \ge \cdots \ge a_\nu.$$

The following lemma can be verified by straightforward manipulations and it will be used to prove that the rows of the triangle $\mathcal{T}^{(1)}$ are unimodal.

Lemma 3. *Let ν and n be integers, such that $\nu \ge 6$ and $0 \le n \le \lfloor \nu/2 \rfloor$. Then*

$$\binom{\nu}{n-2} + \binom{\nu}{n+1} \le \binom{\nu}{n-1} + \binom{\nu}{n+2}.$$

Theorem 4. *For a non-negative integer ν the sequence*

$$\left(T^{(1)}(n, \nu - n)\right)_{0 \le n \le \nu}$$

is unimodal.

Proof. We prove by induction on ν. For $\nu \le 5$ the statement holds. Assume that the statement also holds for some $\nu \ge 6$, that is the νth row of the triangle $\mathcal{T}^{(1)}$ is assumed to be unimodal. We show that this assumption implies the unimodality of row $(\nu + 1)$.

Let us form the sequence $(a_n)_{0 \le n \le \nu+1}$ for which $a_0 = a_{\nu+1} = 0$ and for $1 \le n \le \nu$,

$$a_n = T^{(1)}(n-1, \nu - n + 1) + T^{(1)}(n, \nu - n).$$

The νth row of $\mathcal{T}^{(1)}$ is symmetric, i.e., $T^{(1)}(n, \nu - n) = T^{(1)}(\nu - n, n)$ for each $0 \le n \le \nu$. Consequently, the sequence (a_n) is also symmetric in n. It is also easy to show that the unimodality of the νth row implies the unimodality of the sequence (a_n). Since (a_n) is symmetric and unimodal, its first half is non-decreasing and its second half is non-increasing. It follows that if n is an integer satisfying the condition of Lemma 3, then

$$T^{(1)}(n-1,\nu-n+1)+T^{(1)}(n,\nu-n) \le T^{(1)}(n,\nu-n)+T^{(1)}(n+1,\nu-n-1). \quad (5)$$

Based on Lemma 3 and inequality (5), we obtain that

$$T^{(1)}(n-1,\nu-n+1)+T^{(1)}(n,\nu-n)+\binom{\nu}{n-2}+\binom{\nu}{n+1}$$
$$\le T^{(1)}(n,\nu-n)+T^{(1)}(n+1,\nu-n-1)+\binom{\nu}{n-1}+\binom{\nu}{n+2}. \quad (6)$$

According to the recursion of Corollary 1 with $n+m=\nu$, inequality (6) means that $T^{(1)}(n,\nu-n+1) \le T^{(1)}(n+1,\nu-n)$ holds for $0 \le n \le \lfloor \nu/2 \rfloor$. Since the $(\nu+1)$th row of the triangle is symmetric, we obtain that it is also unimodal. □

2.4. Diagonal sequences of the triangle $\mathcal{T}^{(1)}$

In this subsection, we examine the self-avoiding walks on an $n \times m$ grid with 1 wrong step when m is fixed and n is considered to be a variable. For this reason we deal with the diagonal sequences $(d_m(n))_{n\in\mathbb{N}} = (T^{(1)}(n,m))_{n\in\mathbb{N}}$ of $\mathcal{T}^{(1)}$. These sequences, as we will see, can be described by integer valued polynomials with rational coefficients. We find some properties of the polynomials in order to know more about their nature.

Obviously $d_0(n)$ is the constant 0 polynomial, and in accordance with the proof of Theorem 2 we have $d_1(n) = \binom{n+1}{3} = n(n+1)(n-1)/6$. Theorem 2 implies immediately $d_2(n) = n(n^3+2n^2-n+10)/12$.

Let $h(x) = (x+2)(x+1)(x-1) = x^3+2x^2-x-2$. We will prove the following theorem.

Theorem 5. *For $m \ge 3$ we have*

$$d_m(n) = \frac{1}{A_m} n \cdot (n+3)(n+4)\cdots(n+m)\cdot(h(n)+h(m)),$$

where A_m is $(m+2)(m+1)\cdot(m-1)!$.

Proof. Assume $m \ge 3$. Using the identity $\binom{u}{v} = \binom{u}{u-v}$ of symmetry of binomial coefficients we see

$$d_m(n) = n\binom{n+m}{m-2} + m\binom{n+m}{m+2} = n\frac{(n+m)\cdots(n+3)}{(m-2)!} + m\frac{(n+m)\cdots(n-1)}{(m+2)!}$$
$$= \frac{n\cdot(n+m)\cdots(n+3)}{(m-2)!}\left(1+\frac{(n+2)(n+1)(n-1)}{(m+2)(m+1)(m-1)}\right)$$
$$= \frac{1}{(m+2)(m+1)\cdot(m-1)!} n\cdot(n+3)(n+4)\cdots(n+m)\cdot(h(n)+h(m)).$$

Clearly, $m(m+3)A_m = (m+1)A_{m+1}$. The sequence A_m is registered as A052747 in the On-Line Encyclopedia of Integer Sequences (OEIS [22]). The first few examples for $d_m(n)$ are

$$d_3(n) = \frac{1}{40}n(n+3)(n^3+2n^2-n+38),$$
$$d_4(n) = \frac{1}{180}n(n+3)(n+4)(n^3+2n^2-n+88),$$
$$d_5(n) = \frac{1}{1008}n(n+3)(n+4)(n+5)(n^3+2n^2-n+166).$$

Note that $d_2(n) = n(n^3+2n^2-n+10)/12$ has also a cubic factor, which is exactly $h(n)+h(2)$. Denote $h(n)+h(m)$ by $q_m(n)$, $(m \geq 2)$.

Theorem 6. *The polynomial $q_m(n)$ is irreducible over $\mathbb{Q}$ if $m \geq 2$.*

Proof. Since $q_m(n)$ is monic and $\deg(q_m(n)) = 3$ it is sufficient to show that $q_m(n)$ has no integer zero. On the contrary, assume that there exists an integer L such that $q_m(L) = 0$. Clearly, $L < 0$. Let $L_1 = -L > 0$. Then

$$2(L_1^2+m^2-2) = (L_1-m)(L_1^2+L_1m+m^2-1)$$

follows. The left hand side is positive because $m \geq 2$. Hence $L_1 - m \neq 0$, and

$$2 = (L_1-m)\frac{L_1^2+L_1m+m^2-1}{L_1^2+m^2-2} = (L_1-m)\left(1+\frac{L_1m+1}{L_1^2+m^2-2}\right).$$

The integer factor $L_1 - m$ must be positive since the second factor is positive. If $L_1 - m = 1$, then the second factor is 2. This is possible only when $m = -2$ or $m = 1$, a contradiction. Note that $q_1(n) = h(n)$ is clearly not irreducible. The case $L_1 - m \geq 2$ is also a contradiction, because the second factor is greater than 1. □

3. Explicit formula for the case $w = 2$ on the $n \times m$ grid

The problem becomes more and more complicated if the number w of wrong steps is increased. In this section, we examine the case of $w = 2$. Figures 2 and 3 give all the 1, 2, and 11 walks on the 1×2 grid, 2×2 grid, and 3×2 grid, respectively.

First, we prepare the main theorem of this section, which provides an explicit formula for $T^{(2)}(n,m)$. Define the univariate polynomials

$$\pi_0(x) = \frac{x^2+3x-2}{2}, \quad \pi_1(x) = \frac{x^2+7x-6}{2}, \quad \pi_2(x) = 3(x-1),$$
$$\pi_3(x) = \frac{x^2-x-2}{2}, \quad \pi_4(x) = \frac{x^2-5x+8}{2}. \tag{7}$$

In the next theorem, we assume that $n \geq 1$ and $m \geq 1$ hold for the two sizes of the grid we investigate. Otherwise we cannot reach the point (n,m) from

0

0 0

0 0 0

0 0 0 0

0 0 2 0 0

0 1 11 11 1 0

0 6 42 48 42 6 0

0 21 129 163 163 129 21 0

0 56 339 478 510 478 339 56 0

FIGURE 8. Triangle $\mathcal{T}^{(2)}$

the origin with two error steps. That $T^{(2)}(0,m) = T^{(2)}(n,0) = 0$ is trivially true.

Theorem 7. *The number of self-avoiding walks with $w = 2$ wrong steps on an $n \times m$ grid with $n, m \in \mathbb{N}^+$ is*

$$T^{(2)}(n,m) = -4 + \sum_{j=0}^{4} \pi_j(n)\binom{n+m-1}{n+4-j} + \sum_{j=0}^{4} \pi_j(m)\binom{n+m-1}{m+4-j}. \qquad (8)$$

Similarly to the previous section we can arrange the values of $T^{(2)}(n,m)$ in triangular shape $\mathcal{T}^{(2)}$ as follows in Fig. 8.

Proof. In the proof, we exploit the symmetry between the two parameters n and m. First, suppose that $m = 1$. Then formula (8) simplifies to $\binom{n+1}{5}$, which is correct because there exist $n+1$ vertical edges in the grid, and we must choose 5 of them, 3 for north steps, and 2 for south steps (in the obvious order).

In the sequel, we assume that $n \geq 2$, $m \geq 2$. Suppose even that the first wrong step is horizontal: $(i,j) \longrightarrow (i-1,j)$, where $1 \leq i \leq n$, $1 \leq j \leq m-1$. The step before was clearly $(i,j-1) \longrightarrow (i,j)$. We split the rather technical proof into 3 parts in accordance with the continuation of the possible walks. The statement is obtained by summing the cases. The 3 cases are described here. After the wrong step

(I). we proceed by $(i-1,j) \longrightarrow (i-1,j+1)$, and then never leave the rectangle given by this vertex and (n,m);

(II). we proceed by $(i-1,j) \longrightarrow (i-1,j+1)$, and then somewhere we come down under the line $y = j+1$ to have the second, now vertical error step;

(III). we make the second horizontal error step somewhere from the line $x = i-1$.

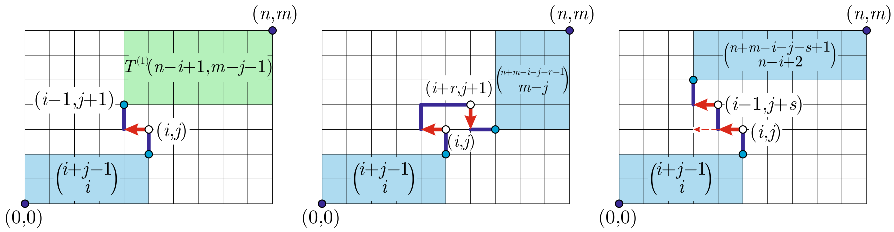

FIGURE 9. Walks with two wrong steps

Figure 9 helps to understand this separation, moreover, it flashes the way of computations. The precise description is provided only in case (I), which is the hardest one, for the other two points we give hints and indicate the crucial arguments only.

Case (I). Denote by $T_I^{(2)} = T_I^{(2)}(n,m)$ the number of walks with two errors under the conditions of (I). Then applying (1) and (2) we have

$$\begin{aligned}
T_I^{(2)} &= \sum_{i=1}^{n}\sum_{j=1}^{m-1} T^{(0)}(i,j-1)T^{(1)}(n-i+1,m-j-1)\\
&= \sum_{i=1}^{n}(n-i+1)\sum_{j=1}^{m-1}\binom{(n+m-i)-j}{n-i+3}\binom{(i-1)+j}{i}\\
&\quad+\sum_{j=1}^{m-1}(m-j-1)\sum_{i=1}^{n}\binom{(n+m-j)-i}{m-j+1}\binom{(j-1)+i}{j-1}\\
&= \sum_{i=1}^{n}(n-i+1)\binom{n+m}{n+4}+\sum_{j=1}^{m-1}(m-j-1)\left(\binom{n+m}{m+1}-\binom{n+m-j}{m-j+1}\right).
\end{aligned}$$

At the last equality we used Lemma 1 for both inner sums. Obviously,

$$\sum_{i=1}^{n}(n-i+1)\binom{n+m}{n+4} = \binom{n+m}{n+4}\sum_{i=1}^{n}(n-i+1) = \binom{n+m}{n+4}\frac{n(n+1)}{2},$$

similarly

$$\sum_{j=1}^{m-1}(m-j-1)\binom{n+m}{m+1} = \binom{n+m}{m+1}\frac{(m-2)(m-1)}{2}.$$

For the remaining term we apply again Lemma 1 as follows.

$$\begin{aligned}
\sum_{j=1}^{m-1}(m-j-1)\binom{n+m-j}{m-j+1} &= (m-1)\sum_{j=1}^{m-1}\binom{n+m-j}{n-1}-\sum_{j=1}^{m-1}\binom{j}{1}\binom{n+m-j}{n-1}\\
&= (m-1)\left(\binom{n+m}{n}-(n+1)\right)
\end{aligned}$$

$$-\left(\binom{n+m+1}{n+1} - nm - (m+1)\right)$$
$$= (m-1)\binom{n+m}{n} - \binom{n+m+1}{n+1} + (n+2).$$

Hence, expressing the lower index in the binomial coefficients as a function of n if necessary we have

$$T_I^{(2)} = \frac{n(n+1)}{2}\binom{n+m}{n+4} + \frac{(m-2)(m-1)}{2}\binom{n+m}{n-1}$$
$$-(m-1)\binom{n+m}{n} + \binom{n+m+1}{n+1} - (n+2).$$

Case (II). The number of corresponding walks is

$$T_{II}^{(2)} = \sum_{i=1}^{n-2}\sum_{j=1}^{m-1} T^{(0)}(i,j-1)\left(T^{(0)}(n-(i-2),m-j) + \cdots + T^{(0)}(0,m-j)\right).$$

The method we used for Case (I) is applicable here as well, finally, we obtain

$$T_{II}^{(2)} = (n-2)\binom{n+m-1}{n-1} - 2\binom{n+m-1}{n-2} + n.$$

Case (III). Now, turn our attention to

$$T_{III}^{(2)} = \sum_{i=2}^{n}\sum_{j=1}^{m-1} T^{(0)}(i,j-1)$$
$$\left(T^{(0)}(n-(i-2),m-(j+1)) + \cdots + T^{(0)}(n-(i-2),0)\right),$$

which simplifies to

$$T_{III}^{(2)} = (n-1)\binom{n+m+2}{n+4}.$$

In total,

$$T^{(2)}(n,m) = T_I^{(2)}(n,m) + T_{II}^{(2)}(n,m) + T_{III}^{(2)}(n,m)$$
$$+T_{I^\star}^{(2)}(n,m) + T_{II^\star}^{(2)}(n,m) + T_{III^\star}^{(2)}(n,m),$$

where $T_{I^\star}^{(2)}(n,m) = T_I^{(2)}(m,n)$, etc. If one uses the functions of n in the lower index of the binomial coefficients everywhere, then the following Table 1 collects the situations and the coefficients of the corresponding binomial coefficients in $T^{(2)}(n,m)$. The upper indices are $n+m-1$, $n+m$, $n+m+1$, $n+m+2$, while the lower indices are $n-4,\ldots,n+4$.

Now use the identity $\binom{u}{v} = \binom{u-1}{v-1} + \binom{u-1}{v}$, successively if necessary, and after simplification we obtain the coefficient polynomials (7). Note that the smallest lower index will be $n-5$. Thus, the proof is complete. □

TABLE 1. The coefficients $\pi_j(x)$ of the equation (8) in Theorem 7

	$n-4$	$n-3$	$n-2$	$n-1$	n	$n+1$	$n+2$	$n+3$	$n+4$
$n+m-1$			-2	$n-2$	$m-2$	-2			
$n+m$	$\frac{m(m+1)}{2}$			$\frac{(m-2)(m-1)}{2}$	$-(n+m-2)$	$\frac{(n-2)(n-1)}{2}$			$\frac{n(n+1)}{2}$
$n+m+1$					1	1			
$n+m+2$			$m-1$						$n-1$

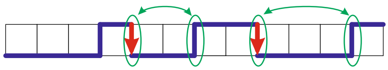

FIGURE 10. A walk on the 12×1 grid with $w = 2$ wrong steps

4. Walks on the $n \times 1$ and $n \times 2$ grids

4.1. Walks on the $n \times 1$ grid

At the beginning of the proof of Theorem 2 we showed that $T^{(1)}(n,1) = \binom{n+1}{3}$. If we allow w error steps on an $n \times 1$ grid, then using analogous argument we can immediately give the number of possible self-avoiding walks for arbitrary w (see Fig. 10).

Theorem 8. *Let n be a positive integer, and assume $0 \le w \le \lfloor n/2 \rfloor$. The number of self-avoiding walks with w wrong steps on an $n \times 1$ grid is*

$$T^{(w)}(n,1) = \binom{n+1}{2w+1}.$$

We mention that the sequences $\left(T^{(w)}(n,1)\right)_{n=0}^{\infty}$ appear in OEIS if $0 \le w \le 49$. These are (using the notation of OEIS) the sequences of binomial coefficients $C(n,1)$, $C(n,3)$, $C(n,5)$, ..., $C(n,99)$, respectively. The first few ones are fitted up with several combinatorial examples, but neither of them is related to self-avoiding walks. The others (most of them) are without any combinatorial background in OEIS.

4.2. Walks on the $n \times 2$ grid

In this section, we derive the number of self-avoiding walks with arbitrary w wrong steps on an $n \times 2$ grid recursively ($n \in \mathbb{N}^+$). We mention that w can not exceed n. Along this section, for brevity we will use the notation $T_n^{(w)} := T^{(w)}(n,2)$.

After introducing a new array we present the main theorem, then we define a system of recurrence sequences to describe the self-avoiding walks, and finally we prove the theorem by the help of the system.

Let the integers b_n^w be defined for $n \in \mathbb{N}$ and $w \in \mathbb{Z}$ as follows in Fig. 11. Let $b_n^w = 0$, if $w < 0$ or $w \ge n$, and put $b_1^0 = 1$, $b_2^0 = 2$, $b_2^1 = 1$. The other values can be determined by applying

$$b_n^w = 2b_{n-1}^w + 2b_{n-1}^{w-1} - b_{n-2}^w - b_{n-2}^{w-1} + b_{n-3}^{w-1} - 2b_{n-3}^{w-2}, \quad n \ge 3,\ 0 \le w \le n-1. \tag{9}$$

We also introduce the function $b(n,w) = b_{n+1}^w - b_{n-1}^{w-1}$ for $n \ge 2$.

0

1 0

2 1 0

3 5 2 0

4 14 11 4 0

5 30 40 26 8 0

6 55 114 109 60 16 0

7 91 274 363 286 136 32 0

8 140 581 1031 1075 724 304 64 0

Figure 11. Triangle of b_n^w

1

3 1

6 4 2

10 13 11 4

15 34 42 26 8

21 75 129 113 60 16

28 146 339 394 294 136 32

36 259 790 1182 1147 740 304 64

45 428 1673 3160 3834 3178 1816 672 128

Figure 12. Triangle $\mathcal{T}_{(2)}^{(w)}$

Theorem 9. *The number of self-avoiding walks with w wrong steps on an $n \times 2$ grid is recursively given by*

$$T_n^{(w)} = T_{n-1}^{(w)} - T_{n-2}^{(w-1)} + b(n,w), \quad 2 \leq n,\ 0 \leq w \leq n \tag{10}$$

with the initial values $T_0^{(0)} = 1$, $T_1^{(0)} = 3$, $T_1^{(1)} = 1$, furthermore, $T_n^{(-1)} = T_n^{(n+1)} = 0$ holds for any $n \geq 0$.

Similarly to the previous sections we can arrange the values of $T_n^{(w)}$ in triangular shape $\mathcal{T}_{(2)}^{(w)}$, where the wth entry of row n is equal to $T_n^{(w)}$ (see Fig. 12).

In this section, a domino always means a vertical one, i.e., its size is 1×2. Let n_1 be a positive integer less than n. The domino corresponding to the points $(n_1 - 1, 0)$ and $(n_1, 2)$ is called the tail of the $n_1 \times 2$ grid. As a self-avoiding walk crosses a domino it draws a pattern onto the domino. Sometimes

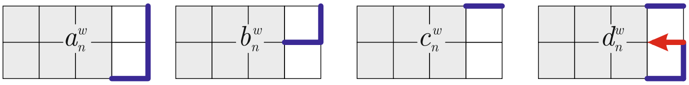

FIGURE 13. Types of tails of self-avoiding walks on the $n \times 2$ grid

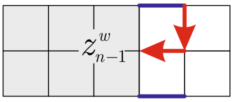

FIGURE 14. A z-type semi-tail on the $n \times 2$ grid

we do not consider the whole pattern but only its so-called essential part (from certain point of view). Studying the possible essential tails on the $n \times 2$ grid (see Figs. 2 and 3) we found four types. These are denoted by type a, b, c, and d, and illustrated in Fig. 13. Let a_n^w, b_n^w, c_n^w, and d_n^w denote the number of the self-avoiding walks on an $n \times 2$ grid when the type of their tails is a, b, c, and d, respectively. Take, for example, the first type (i.e., type a) in Fig. 13. The essential part of the self-avoiding walk starts at $(n-1, 0)$, and it is irrelevant whether we came here from $(n-2, 0)$ or from $(n-1, 1)$.

It is easy to see that a domino can contain zero, one, two, or three wrong steps of a self-avoiding walk. The case of three wrong steps can not occur on the tail of the $n \times 2$ grid because the walk ends at $(n, 2)$, but it can be a tail of the $(n-1) \times 2$ grid (if our purpose is to investigate the $n \times 2$ grid). We say that this has type z, and we call it the semi-tail of the $n \times 2$ grid (see Fig. 14). Simply the semi-tail is the last but one domino, which assists us to describe a system of equations. Let $z_{n_1}^w$ denote the number of self-avoiding walks on an $n_1 \times 2$ grid when the last domino has type z and we finish the walk at the grid point $(n_1, 0)$.

Collecting all walks with the possible tails and occasionally with a z-semi-tail we found recurrence connections among a_n^w, b_n^w, c_n^w, d_n^w, and z_n^w. Figure 15 helps us to explain the nature of the recurrences. For example, the left part of the fifth line of the figure shows how an a-type tail can be transformed into a d-type tail whilst the grid is expanded by one more domino that the walk contains one more wrong step (In short, $a_{n-1}^{w-1} \to d_n^w$).

Summarizing and rewriting the table into the form of Fig. 16, we obtain the complete system of recurrences. Leaving the graphics mode we extract the observations in

Lemma 4. *The number of self-avoiding walks with w wrong steps on an $n \times 2$ grid is given by the system of the recurrence relations*

$$a_n^w = a_{n-1}^w + z_{n-1}^w + b_{n-1}^{w-1} + c_{n-1}^{w-2},$$

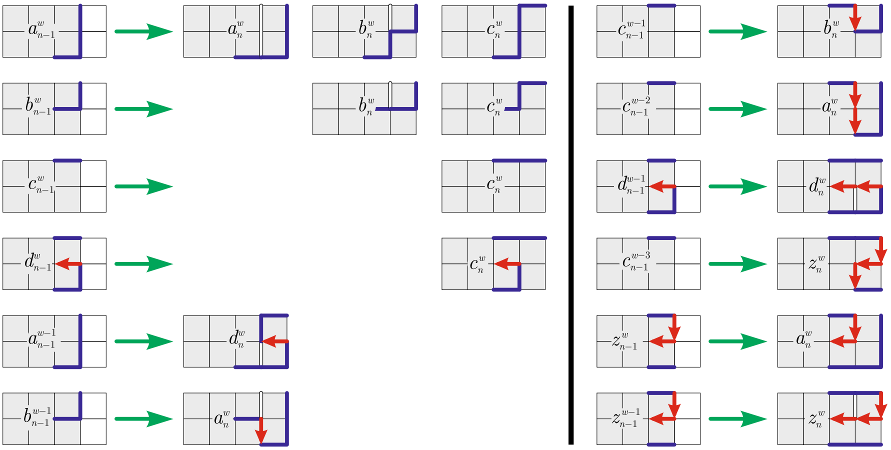

FIGURE 15. Recurrence table for self-avoiding walks on the $n \times 2$ grid

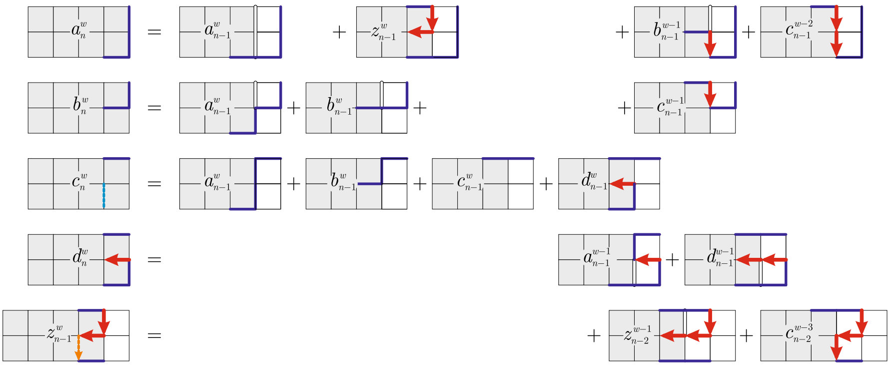

FIGURE 16. System of the recurrences of the tails on the $n \times 2$ grid

$$
\begin{aligned}
b_n^w &= a_{n-1}^w + b_{n-1}^w + c_{n-1}^{w-1}, \\
c_n^w &= a_{n-1}^w + b_{n-1}^w + c_{n-1}^w + d_{n-1}^w, \\
d_n^w &= a_{n-1}^{w-1} + d_{n-1}^{w-1}, \\
z_{n-1}^w &= z_{n-2}^{w-1} + c_{n-2}^{w-3},
\end{aligned} \tag{11}
$$

where $2 \leq n$, $0 \leq w \leq n$ *and*

$$T_n^{(w)} = a_n^w + b_n^w + c_n^w + d_n^w = c_{n+1}^w$$

with zero initial values except $a_0^0 = 1$, $a_1^0 = b_1^0 = c_1^0 = 1$, *and* $d_1^1 = 1$.

Now we turn our attention to the proof of Theorem 9.

Proof of Theorem 9. First, we eliminate the terms z_n^w from the system (11). For this reason we express z_{n-1}^w from the first equation, shift the indices and replace the three terms of the last equation. After some simplifications we obtain the first new equation

$$a_n^w = a_{n-1}^w + a_{n-1}^{w-1} + b_{n-1}^{w-1} - a_{n-2}^{w-1} - b_{n-2}^{w-2} + c_{n-1}^{w-2}.$$

The second term we eliminate is d_n^w. Combining the third and the fourth equations of (11) we have the second new equation, which is the last item of the system

$$\begin{aligned} a_n^w &= a_{n-1}^w + a_{n-1}^{w-1} + b_{n-1}^{w-1} - a_{n-2}^{w-1} - b_{n-2}^{w-2} + c_{n-1}^{w-2}, \\ b_n^w &= a_{n-1}^w + b_{n-1}^w + c_{n-1}^{w-1}, \\ c_n^w &= c_{n-1}^w + a_{n-1}^w + b_{n-1}^w + c_{n-1}^{w-1} - b_{n-2}^{w-1} - c_{n-2}^{w-1}. \end{aligned}$$

Combine now the first two equations, which results in $a_n^w = a_{n-1}^w + b_n^{w-1} - a_{n-2}^{w-1} - b_{n-2}^{w-2}$, and in parallel subtract the second equation from the third one to obtain $c_n^w = b_n^w + c_{n-1}^w - b_{n-2}^{w-1} - c_{n-2}^{w-1}$, or equivalently $c_n^{w-1} = b_n^{w-1} + c_{n-1}^{w-1} - b_{n-2}^{w-2} - c_{n-2}^{w-2}$. Thus, we arrive at the system

$$\begin{aligned} a_n^w &= a_{n-1}^w + c_n^{w-1} - c_{n-1}^{w-1} - a_{n-2}^{w-1} + c_{n-2}^{w-2}, \\ b_n^w &= a_{n-1}^w + b_{n-1}^w + c_{n-1}^{w-1}, \\ c_n^w &= b_n^w + c_{n-1}^w - b_{n-2}^{w-1} - c_{n-2}^{w-1}. \end{aligned}$$

Eliminate now the term a_n^w from the second equality, shift it, and then we have

$$\begin{aligned} b_n^w &= 2b_{n-1}^w - b_{n-2}^w + 2c_{n-1}^{w-1} - 2c_{n-2}^{w-1} - b_{n-2}^{w-1} + b_{n-3}^{w-1} + 2c_{n-3}^{w-2}, \\ c_n^w &= b_n^w + c_{n-1}^w - b_{n-2}^{w-1} - c_{n-2}^{w-1}. \end{aligned}$$

Finally, we see $c_{n-1}^{w-1} - c_{n-1}^{w-2} + c_{n-3}^{w-2} = b_{n-1}^{w-1} - b_{n-3}^{w-2}$ (from the second equation), and using it we conclude the recurrence

$$b_n^w = 2b_{n-1}^w - b_{n-2}^w + 2b_{n-1}^{w-1} - b_{n-2}^{w-1} + b_{n-3}^{w-1} - 2b_{n-3}^{w-2}.$$

The initial values of the recurrence sequences are obvious. □

In the following, we highlight the first five sequences depending on the numbers of the wrong steps. These are the left-down diagonal sequences of Triangle $\mathcal{T}_{(2)}^{(w)}$ in Fig. 12. Only the first one has appeared in OEIS yet.

$$\begin{aligned} (T_n^{(0)})_{n=0}^{\infty} &= (1, 3, 6, 10, 15, 21, 28, 36, 45, 55, 66, 78, 91, \ldots), \\ (T_n^{(1)})_{n=0}^{\infty} &= (0, 1, 4, 13, 34, 75, 146, 259, 428, 669, 1000, 1441, 2014, \ldots), \\ (T_n^{(2)})_{n=0}^{\infty} &= (0, 0, 2, 11, 42, 129, 339, 790, 1673, 3278, 6024, 10493, 17468, \ldots), \\ (T_n^{(3)})_{n=0}^{\infty} &= (0, 0, 0, 4, 26, 113, 394, 1182, 3160, 7691, 17300, 36384, 72214, \ldots), \end{aligned}$$

$$(T_n^{(4)})_{n=0}^{\infty} = (0, 0, 0, 0, 8, 60, 294, 1147, 3834, 11400, 30845, 77118, 180176, \ldots).$$

Remark 3. In the case of an $n \times 2$ grid the number of all self-avoiding walks is equal to the sum of self-avoiding walks with zero, one, two, ..., and n wrong steps, so the sum of entries in the nth row of triangle $\mathcal{T}_{(2)}^{(w)}$. This sum sequence is

$$(\xi_n)_{n=0}^{\infty} = (1, 4, 12, 38, 125, 414, 1369, 4522, 14934, 49322, 162899, 538020, \ldots),$$

and it also has a recursive description

$$\xi_n = 4\xi_{n-1} - 3\xi_{n-2} + 2\xi_{n-3} + \xi_{n-4}, \quad n \geq 4.$$

(See [1].) Since (ξ_n) appears in OEIS as sequence A006192 with the explanation "number of nonintersecting (or self-avoiding) rook paths joining opposite corners of $3 \times n$ board" it means an independent verification for our result. Note that the expression "$3 \times n$ board" above is equivalent to the case $n \times 2$ in our interpretation.

5. Conclusion

Most of the results of Madras in [16] have been proved not only for squares, but also for arbitrary d-dimensional hyper-cubic lattices. The question naturally arises whether our results could be extended to higher dimensional rectangular cuboids. Our proof techniques in Theorems 2 and 7, which gave closed formulas for the number of self-avoiding walks crossing a two dimensional rectangular grid, would probably work in higher dimensions as well, but there are so many distinct cases to consider that the proof would become too inconvenient as the dimension increases. We encountered similar difficulties when considering three or more wrong steps.

Our other results show a similarly large increase in the number of cases to be treated when we increase one of the parameters. For example, in Sect. 4, increasing the width of the rectangle to $m > 2$ makes it excessively difficult to handle special cases when counting walks with an arbitrary number of wrong steps. Recently, Nyblom in [19] has also studied the same domains as we do in Sect. 4, but he counts different subsets of the self-avoiding walks. In [20], Nyblom similarly faces increasing challenges as he increases the width of the rectangles.

Acknowledgements

While the difficulties of dealing with such a wide range of special cases have limited our current study, we would expect that with newer methods our results could be extended. The development of such methods could be a task for further research. For L. Szalay the research was supported by Hungarian National Foundation for Scientific Research Grant No. 128088, and No. 130909, and by the Slovak Scientific Grant Agency VEGA 1/0776/21. The authors are grateful the anonymous referee for the valuable suggestions, and we would like to thank him/her for the useful remarks and questions.

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Declarations

Conflict of interest The authors declare that they have no conflict of interest.

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