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SELF-AVOIDING WALKS ON LATTICE STRIPS^{*}

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ABSTRACT. We study self-avoiding walks (SAWs) on restricted square lattices, more precisely on the lattice strips $\mathbb{Z} \times \{-1, 0, 1\}$ and $\mathbb{Z} \times \{-1, 0, 1, 2\}$. We obtain the value of the connective constant for the $\mathbb{Z} \times \{-1, 0, 1\}$ lattice in a new shorter way and deduce close bounds for the connective constant for the $\mathbb{Z} \times \{-1, 0, 1, 2\}$ lattice. Moreover, for both lattice strips we find close lower and upper bounds for the number of SAWs of length n by using the connective constant. Additionally, we present a transformation of SAWs on the square lattice to a special kind of walks on the honeycomb lattice. By using H. Duminil-Copin and S. Smirnov's results for SAWs on the honeycomb lattice we present non-rigorous ways by which close bounds for the number of SAWs and for the connective constant of the non-restricted square lattice could eventually be obtained without the need of long computer computations.

1. Introduction. A self-avoiding walk (SAW) is a path that does not self-intersect, i.e., it does not pass through a given point more than once. SAWs were introduced by Flory, a theoretical chemist, in order to model the behaviour

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of linear polymers in dilute solutions ([6, p. 672]). They quickly became an intriguing combinatorial problem for mathematicians and an interesting computational problem for computer scientists (see [10]).

In this paper we study SAWs on the two-dimensional square lattice.

Definition 1.1. A self-avoiding walk (SAW) of length n is a sequence of points (w_0, w_1, \dots, w_n) where $w_0 = (0, 0)$ and $w_i = (x_i, y_i)$ (x_i and y_i integers), such that no point repeats itself and $|x_{i+1} - x_i| + |y_{i+1} - y_i| = 1$ for all i , where $i \in \{0, 1, \dots, n-1\}$. We define the move from point w_i to point w_{i+1} to be called a step.

For the lattice $\mathbb{Z} \times \{x, x+1, \dots, y\}$ we denote the number of SAWs of length n with $c_{[x,y]n}$. If x and y are, respectively, minus and plus infinity we just write c_n .

An exact formula for $c_{[x,y]n}$ has only been obtained for $c_{[0,1]n}$ ([2, 9, 13]).

Theorem 1.2 ([13]). For $n \geq 2$, the number of SAWs of length n on the grid $\mathbb{Z} \times \{0, 1\}$ is

$$c_{[0,1]n} = 8F_n - \delta_n$$

where F_n is the n^{th} Fibonacci number and $\delta_n = 4$ if n is odd and $\delta_n = n$ otherwise.

It is conjectured $c_n \sim A\mu^n n^v$, where A , μ and v are constants. The most studied one of them is the connective constant μ .

Definition 1.3. The limit $\lim_{n \rightarrow \infty} \sqrt[n]{c_n}$ is called the connective constant and we denote it by $\mu_{\mathbb{Z} \times \mathbb{Z}}$. For the lattice strip $\mathbb{Z} \times \{x, x+1, \dots, y\}$ we define the connective constant analogously and denote it by $\mu_{[x,y]}$.

The connective constant could be proven to exist and to be finite by using Fekete's lemma and that $c_n c_m \geq c_{n+m}$. There are also strong bounds for c_n using $\mu_{\mathbb{Z} \times \mathbb{Z}}$ in [8]. However, even the value for $\mu_{\mathbb{Z} \times \mathbb{Z}}$ is not known.

A way one could obtain μ is to observe when does the series of the generating function (for a background on generating functions see [11])

$$G(t)_{[x,y]} = 1 + c_{[x,y]1}t + c_{[x,y]2}t^2 + \dots$$

converge. $G(t)_{[x,y]}$ has been found only when $x = 0$ and $y = 1$ (see [13]) and when $x = -1$ and $y = 1$ (see [3]). Respectively, $\mu_{[0,1]}$ equals the golden ratio and $\mu_{[-1,1]} \approx 1.914\dots$

It is a natural idea to try to study increasingly larger lattice strips since if we let the width of the strip go to infinity then we end up at the original problem

for the $\mathbb{Z} \times \mathbb{Z}$ lattice. In 1990 S. Erick and J. Svante obtained the value for the connective constant of all lattice strips on the square lattice with width up to 9 by using the transfer matrix method (see [1]). However, the bigger the lattice, the more computational power is needed and even with modern computers we cannot get very far.

Here, we take a computationally less expensive approach of counting SAWs via the following major breakthrough, made by H. Kesten. He showed that there exists a class of walks called bridges which have the same connective constant as all SAWs on the square lattice (see [7]).

Definition 1.4. *Let us have a self-avoiding walk with coordinates (w_0, w_1, \dots, w_n) , as $w_0 = (0, 0)$. Then a SAW is a bridge if $x_0 < x_j \leq x_n$ for all $j > 0$, where x_i is the x -axis coordinate of the i^{th} point. We use b_n to denote the number of n -step bridges on the $\mathbb{Z} \times \mathbb{Z}$ grid. Kesten showed that $b_n^{\frac{1}{n}}$ converges to $\mu_{\mathbb{Z} \times \mathbb{Z}}$ as $n \rightarrow \infty$. For the lattice strip $\mathbb{Z} \times \{x, x+1, \dots, y\}$ we denote the number of bridges by $b_{[x,y]_n}$. Respectively, we define the generating function of the bridges to be $B(t)_{[x,y]} = \sum_{n=0} b_{[x,y]_n} t^n$.*

Moreover, the above definition can be extended to the hexagonal lattice with the difference that the coordinates x_j will not be integers. In 2010, by using bridges, H. Duminil-Copin and S. Smirnov proved a conjecture by B. Nienhuis that the connective constant on the honeycomb lattice equals $\mu_H = \sqrt{2 + \sqrt{2}}$ (see [5]). In this project we want to apply this result for the square lattice.

In the second and third section of this paper we show an application of counting bridges directly with generating functions. We find $\mu_{[-1,1]}$ in a new shorter way and obtain close lower and upper bounds for $\mu_{[-1,2]}$. Our method yields that $\frac{1}{\mu_{[-1,1]}}$ is the smallest modulus root of the equation $1 - t - 2t^3 - t^4 - 2t^5 - 2t^6 = 0$ and that $2.050 \leq \mu_{[-1,2]} \leq 2.166$. Moreover, the Hammersley-Welsh method (see e.g. [8, p. 57]) allows us to derive close lower and upper bound for $c_{[-1,1]_n}$ and $c_{[-1,2]_n}$ through the use of $\mu_{[-1,1]}$ and $\mu_{[-1,2]}$, respectively. In the end we do not have the exact number of walks but we do have a good idea for their growth rate.

In the fourth section of the paper we present a transformation of n -step SAWs on the square lattice to a special type of walks – SSAWs (semi-self-avoiding walks) on the honeycomb lattice with $2n$ steps (the transformation is bijective). Our interest comes from the fact that the walks on the honeycomb lattice are easier

to describe mathematically, because we know that $\mu_H = \sqrt{2 + \sqrt{2}}$. In addition, we make a conjecture that, on average, a SAW on the square lattice with length n will make approximately $0.6n$ turns for sufficiently large n . Moreover, we propose methods which eventually may yield close bounds for c_n and $\mu_{\mathbb{Z} \times \mathbb{Z}}$ without the need of long computer calculations.

2. The connective constant on the $\mathbb{Z} \times \{-1, 0, 1\}$ lattice.

We prove the following result

$$(1) \quad \mu_{[-1,1]}^n \leq c_{[-1,1]n} \leq \mu_{[-1,1]}^{n+1} ((n+1) + 2(n+1)^2 + 3(n+1)^3 + 2(n+1)^4 + (n+1)^5)$$

for $n \geq 1$ in Appendix B by using the Hammersley-Welsh Method. From the proof one gets as a bonus that $\lim_{n \rightarrow \infty} \sqrt[n]{b_{[-1,1]n}} = \mu_{[-1,1]}$.

Therefore, the problem translates to counting bridges. To do that we use Zeilberger's Decomposition Method (see [13]) and *irreducible bridges*. Zeilberger's Decomposition Method is an "alphabetical" approach for describing the self-avoiding walk. A generalisation of this method is presented in [12] in order to count up-side SAWs. One divides the SAWs in their basic movements which they perform and for each of them one chooses a symbol to represent it. These symbols become our "letters" of an "alphabet" for creating different "words" (SAWs). For example, our language for the $\mathbb{Z} \times \{-1, 0, 1\}$ grid consists of 3 different two letter combinations allowing us to construct every bridge.

- I_O – denotes an irreducible bridge between an inner and outer line;
- O_O – denotes an irreducible bridge between the two outer lines;
- O_I – denotes an irreducible bridge between an outer and inner line.

The two outer lines are the horizontal lines $y = 1$ and $y = -1$. The inner line is the horizontal line $y = 0$.

We proceed with the explanation of what is an **irreducible bridge**. Whenever we join two bridges of lengths m and n we get another bridge of length $m + n$. As a result, every bridge can be decomposed into *irreducible bridges* (bridges which cannot be decomposed further). However, now a straight line of k right steps is actually k irreducible bridges of length 1 glued to each other. Therefore, for our convenience let us make the following correction in our understanding of what an irreducible bridge will be (this new understanding is used above, when describing the two-letter combinations I_O , O_O and O_I). If we have a line of k irreducible bridges of length 1 and then another irreducible bridge of length bigger than 1, then we will consider all these $k + 1$ irreducible bridges as a single irreducible bridge (see Fig. 1). We will relate to the k right steps in the beginning of the irreducible bridge as its **tail**.

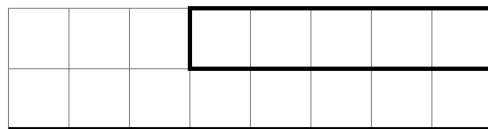


Fig. 1. An O_O irreducible bridge with a tale of length 2

Proposition 2.1. *The following code using O_O , O_I and I_O describes all bridges.*

$$[I_O O_O^* O_I]^* \widetilde{I_O O_O^* r^*}$$

where the symbol $'^*$ ' is an indefinite superscript (≥ 0), the tilde indicates that the movement may not be executed and r is a step to the right.

The tilde and star can be considered as the “punctuation” needed for our “language”.

In order to deduce the generating function of all bridges we need to find the generating function for each of the types of irreducible bridges — O_O , O_I , and I_O .

In this section we will obtain the generating function of the most complex one, the O_O type. Firstly, we derive the generating function of the irreducible bridges without a tail. Let us assume we are on the higher outer line (because the grid is symmetric it does not matter). The irreducible bridges follow a certain pattern. For $k \geq 0$ they always consists of $k + 1$ steps to the right followed by a step down and k steps to the left. Then we have another step down and k steps to the right. The generating function is:

$$\frac{t^3}{1 - t^3}$$

We can add the tail by multiplying the generating function by $\frac{1}{1 - t}$:

$$G_{OO} = \frac{t^3}{1 - t - t^3 + t^4}$$

We find the generating functions of the other types of irreducible bridges similarly (Table 1).

We need to calculate the generating function of O_O^* . Since O_O^* is just an indefinite number of O_O irreducible bridges glued to each other, the generating function is

$$G(t)_{OO^*} = \frac{1}{1 - \frac{t^3}{1 - t - t^3 + t^4}} = \frac{1 - t - t^3 + t^4}{1 - t - 2t^3 + t^4}$$

Table 1

Irred. Bridge	Generating function
O_I	$\frac{t^2}{(1-t)} = t^2 + t^3 + t^4 + t^5 + \dots$
I_O	$\frac{2t^2}{(1-t)} = 2t^2 + 2t^3 + 2t^4 + 2t^5 + \dots$
O_O	$\frac{t^3}{1-t-t^3+t^4} = t^3 + t^4 + t^5 + 2t^6 + \dots$

Hence,

$$B(t)_{[-1,1]} = \frac{1}{1 - G(t)_{IO}G(t)_{OO^*}G(t)_{OI}}(1 + G(t)_{IO}G(t)_{OO^*})G(t)_{u^*}$$

$$= \frac{1-5t+12t^2-22t^3+35t^4-47t^5+56t^6-58t^7+49t^8-37t^9+25t^{10}-11t^{11}+2t^{12}}{1-6t+15t^2-24t^3+35t^4-48t^5+53t^6-46t^7+31t^8-16t^9+4t^{10}+10t^{11}-17t^{12}+10t^{13}-2t^{14}}$$

Hence, we have obtained our desired generating function. In order to deduce the value of $\mu_{[-1,1]}$, we find the smallest modulus root of the denominator of $B(t)_{[-1,1]}$, and take its reciprocal:

Proposition 2.2. *The value of the connective constant on the $\mathbb{Z} \times \{-1, 0, 1\}$ lattice is approximately:*

$$\mu_{[-1,1]} \approx \frac{1}{0.522295} \approx 1.914.$$

However, if we look carefully, the real structure of the SAW is encoded in the generating function of $[I_O O_O^* O_I]^*$. One could only calculate that generating function and it turns out that the desired root is really there. The denominator reduces to the simple polynomial $1 - t - 2t^3 - t^4 - 2t^5 - 2t^6$.

3. Self-avoiding walks on the $\mathbb{Z} \times \{-1, 0, 1, 2\}$ grid. In Appendix B we prove that

$$(2) \quad \mu_{[-1,2]}^n \leq c_{[-1,2]n} \leq \mu_{[-1,2]}^{n+1} P(n)$$

where $P(n) = (n+1)+2(n+1)^2+3(n+1)^3+4(n+1)^4+3(n+1)^5+2(n+1)^6+(n+1)^7$ for $n \geq 1$ by using the Hammersley-Welsh Method. It yields as a bonus that $\lim_{n \rightarrow \infty} \sqrt[n]{b_{[-1,2]n}} = \mu_{[-1,2]}$.

We again introduce a similar linguistic approach to the problem and use the same definition for an irreducible bridge. We use the same irreducible bridges

of types O_O , O_I , I_O , however, we do introduce one more: I_I will denote an irreducible bridge between the two inner lines, because now we have two outer ($y = 2$ and $y = -1$) and two inner ($y = 0$ and $y = 1$) lines.

Proposition 3.1. *Every bridge can be encoded in the following way:*

$$[I_I^* I_O O_O^* O_I]^* I_I^* \widetilde{I_O O_O^*} r^*.$$

Hence, the problem translates to finding the generating function for each of the four types of irreducible bridges. However, on the $\mathbb{Z} \times \{-1, 0, 1, 2\}$ lattice, SAWs have much more freedom and thus, their behaviour is harder to describe. If we want to count all bridges, we will have to count SAWs, such as the one shown in Fig. 2, and in some way include it in our generating function. The calculations soon becomes quite unpleasant. Nevertheless, we can use our method to derive close bounds for the connective constant. For example, if we count parts of the irreducible bridges of each type (O_O , I_O , ...) and analyse the resulting generating function, we will obtain a lower bound for the connective constant. The same reasoning is used for for the upper bound.

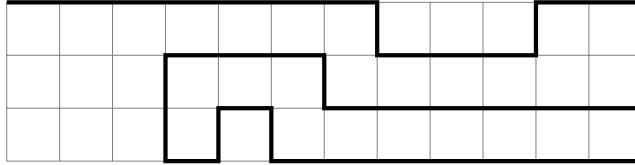


Fig. 2. An O_O irreducible bridge with a tail of length 2

We show examples of how we can obtain “good” bounds for the connective constant, although if one makes more calculations, even better bounds could be found.

3.1. Lower bound for the connective constant. For our lower bound we need to count part of the irreducible bridges for each of the types O_O , O_I , I_I and I_O . Let us count only those which do not make a step to the left. Hence, we will count right-side walks, whose first step is to the right. We present a table with the generating functions:

Therefore, the generating function of all right-side SAWs, which start with a right step is:

$$\frac{1 - t + t^2 + t^3 - t^4}{1 - 2t + t^3 - 2t^4 - t^5} = 1 + t + 3t^2 + 6t^3 + 12t^4 + 24t^5 + \dots .$$

The radius of convergence is approximately 0.487645.

Table 2

Irred. Bridge	Generating function
I_I	$\frac{t^2}{1-t} = t^2 + t^3 + t^4 + t^5 \dots$
O_I	$\frac{t^2+t^3}{(1-t)} = t^2 + 2t^3 + 2t^4 + 2t^5 + \dots$
I_O	$\frac{t^2+t^3}{(1-t)} = t^2 + 2t^3 + 2t^4 + 2t^5 + \dots$
O_O	$\frac{t^4}{(1-t)} = t^4 + t^5 + t^6 + t^7 + \dots$

Corollary 3.2. *The following lower bound for the connective constant is true:*

$$\frac{1}{0.487645} \approx 2.050 \leq \mu_{[-1,2]}.$$

3.2. Upper bound for the connective constant. We proceed with the upper bound. Through exhaustive search we discover that there are 2 types of irreducible bridges, which follow certain patterns:

We may have a tail. Then we have a step to the right and respectively one, two or three steps upward or downward depending on which type of irreducible bridge we are performing – we will call these irreducible bridges *simple* (Fig. 3).

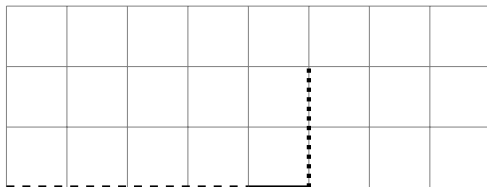


Fig. 3. A simple O_I irreducible bridge. We have a tail of length four followed by a step to the right. Afterwards we have two steps upwards

The other pattern is as follows. We assume we are on one of the two lower lines, parallel to the x -axis ($y = 0$ and $y = -1$), as the other case is analogical. We may have a tail. Then we have 3 avoidable SAWs on strips with length 1, which go in “opposite” directions, as the first walk goes right (on the strip $\mathbb{Z} \times \{-1, 0\}$), the second one goes left (on the strip $\mathbb{Z} \times \{0, 1\}$), and the third one goes to the right again (on the strip $\mathbb{Z} \times \{1, 2\}$). Their starting and ending points are determined by the type of irreducible bridge. We call these bridges *complicated* (Fig. 4).

First, we examine irreducible bridges of type O_O .

Let us imagine a complicated bridge that starts from the higher outer line. We ignore the tail for now and perform the following operation: do not move the

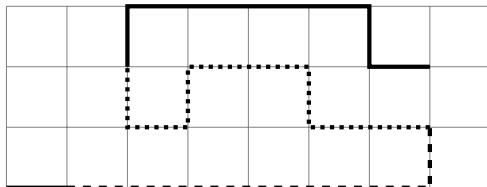


Fig. 4. A complicated O_I irreducible bridge. We have a tail of length 1. Afterwards we have a walk that goes right on the strip $\mathbb{Z} \times \{-1, 0\}$ of length 7. Then a walk that goes left on the strip $\mathbb{Z} \times \{0, 1\}$ of length 8 followed by a walk that goes right on the strip $\mathbb{Z} \times \{1, 2\}$ of length 7

walk that goes right on the grid $\mathbb{Z} \times \{1, 2\}$. However, we add a right step where it ends and place the beginning of the walk that goes left in the end of the added right step and rotate it about its beginning by 180 degrees. It became a walk that goes right. We proceed by adding another right step and at its end we place the beginning of the walk that goes right on the grid $\mathbb{Z} \times \{-1, 0\}$. Hence, we transformed our irreducible bridge without a tail into a walk with two more steps on the grid $\mathbb{Z} \times \{1, 2\}$, as we know the lines on which it starts and ends. (We show an example on Figures 5 and 6.) Notice that we add right steps because otherwise our transformed walk may not be a SAW. Moreover, every irreducible bridge O_O without a tail has a unique transformed walk. However, the inverse is not true.

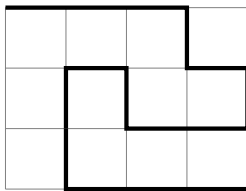


Fig. 5. O_O irreducible bridge without a tail

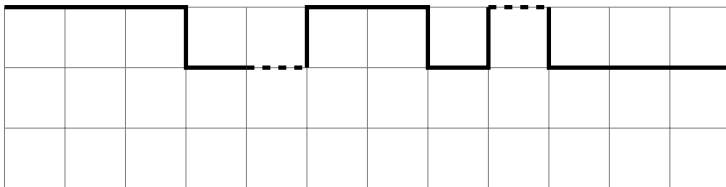


Fig. 6. The bridge from Fig. 5 after the transformation

We now find the generating function of the transformed SAWs. Such a transformed SAW cannot make left steps, it is only on the grid $\mathbb{Z} \times \{1, 2\}$, its starting and ending points are on different lines (beginning on the outer line and ending on the inner one) and the first step is always to the right.

The generating function equals

$$\frac{\frac{t^2}{1-t}}{1 - \frac{t^4}{(1-t)^2}} \frac{1}{1-t} = \frac{t^2}{1 - 2t + t^2 - t^4}.$$

If we divide the above generating function by t^2 (because of the added 2 right steps) we will obtain a generating function whose coefficient in front of the n^{th} power is bigger than or equal to the number of irreducible bridges of type O_O without a tail of length n :

$$\frac{1}{1 - 2t + t^2 - t^4} = 1 + 2t + 3t^2 + 4t^3 + 6t^4 + 10t^5 + \dots .$$

However, as we want to make the coefficients more accurate, we will decrease the coefficients in front of the first 14 powers. (We check by exhaustive search that these coefficients can be decreased.)

$$\begin{aligned} \frac{1}{1 - 2t + t^2 - t^4} &= (1 + 2t + 3t^2 + 4t^3 + 5t^4 + 10t^5 + 17t^6 + 24t^7 + 45t^8 + 72t^9 \\ &\quad + 109t^{10} + 188t^{11} + 301t^{12} + 474t^{13}) \\ &= \frac{t^4 - 2t^5 + t^6 + 4t^7 - 9t^8 + 4t^9 + 7t^{10} - 18t^{11} + 11t^{12} + 12t^{13} + 756t^{14} - 286t^{15} + 301t^{16} + 474t^{17}}{1 - 2t + t^2 - t^4}. \end{aligned}$$

Moreover, we notice that we also counted the simple irreducible bridges in the generating function. (We did not decrease the coefficient in front of the fourth power with 6.) Now we can add the tail by multiplying by $\frac{1}{1-t}$. Hence we will obtain a generating function whose coefficient in front of the n^{th} power is bigger than or equal to the number of irreducible bridges of type O_O with length n .

The other types of irreducible bridges will be considered in Appendix A.

In the end, our calculations yield one “big” generating function. We again look at the “important” part of the code of all bridges:

$$[I_O O_O^* O_I I_I^*]^*.$$

The denominator of the generating function of this part of the code is

$$D(t) = 1 - 12t + 65t^2 - 209t^3 + 434t^4 - 568t^5 + 338t^6 + 305t^7 - 907t^8$$

$$\begin{aligned}
& + 770t^9 + 292t^{10} - 1462t^{11} + 1406t^{12} + 446t^{13} - 3945t^{14} + 13408t^{15} \\
& - 42903t^{16} + 101573t^{17} - 158117t^{18} + 136952t^{19} + 4507t^{20} \\
& - 182921t^{21} + 225943t^{22} - 49787t^{23} - 215357t^{24} + 317489t^{25} \\
& - 108470t^{26} - 314100t^{27} + 801774t^{28} - 1620468t^{29} + 3204285t^{30} \\
& - 4939210t^{31} + 4697564t^{32} - 1024682t^{33} - 3939143t^{34} + 5903640t^{35} \\
& - 3220560t^{36} - 980952t^{37} + 2685716t^{38} - 1510904t^{39} - 162295t^{40} \\
& + 605850t^{41} - 239118t^{42} - 42432t^{43} + 55764t^{44}.
\end{aligned}$$

The radius of convergence is approximately 0.461722.

Corollary 3.3. *The following upper bound for the connective constant is true:*

$$\mu_{[-1,2]} \leq 2.166.$$

4. Transformation of SAWs on the square lattice in walks on the honeycomb lattice. In this section we will present a transformation of SAWs on the square lattice $\mathbb{Z} \times \mathbb{Z}$ to a special kind of walks on the so called honeycomb lattice or hexagonal lattice, but with twice as many steps. We are interested in this transformation because the value of the connective constant for the hexagonal lattice is known and equals $\mu_H = \sqrt{2 + \sqrt{2}}$.

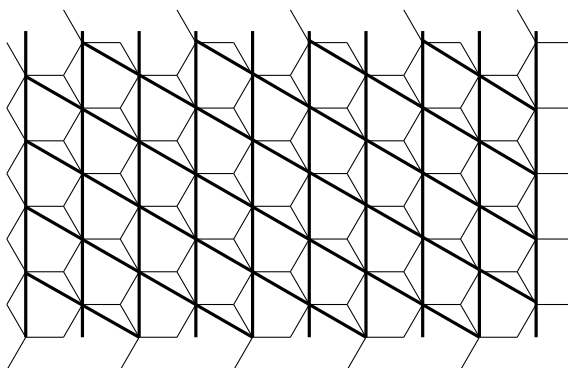


Fig. 7. The square grid analogue drawn over the hexagonal grid

Let us draw a grid of rhombuses onto the hexagonal lattice as shown on Fig. 7. We will refer to this grid as a square lattice as it is analogical.

Now on every step on the square lattice we will superpose two steps on the hexagonal lattice, with whom the step on the square lattice forms an isosceles triangle (Fig. 8).

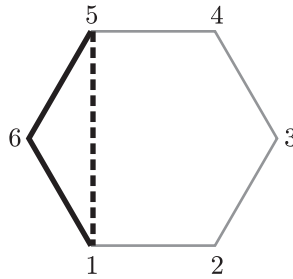


Fig. 8. Mapping a step on the square lattice to two steps on the hexagonal lattice

We will analyse what kind of characteristics do walks on the hexagonal lattice have, when they are transformed from a SAW on the square lattice.

- The walk starts from a point through which the square lattice passes.
- It is not allowed the steps between points 1 - 2 and 2 - 3 (Fig. 8) for a given hexagon to occur consecutively, as we cannot superpose a step on the square lattice.
- Consider the configuration of two hexagons on Fig. 9. If on the square

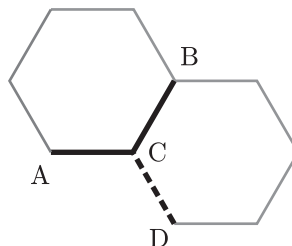


Fig. 9. Situation of intersection

lattice we made steps from point A to point D and then to point B, on the hexagonal lattice we will have passed through the segment C - D twice. The same would happen if the SAW goes in the opposite direction. This intersection is the only one for this type of walks as every step on the square lattice has its unique pair of steps on the hexagonal lattice.

Definition 4.1. A walk with the above properties will be called a semi-self-avoiding walk (SSAW).

Theorem 4.2. *There is a bijective correspondence between SAWs from the square lattice with length n and SSAWs on the hexagonal lattice with length $2n$.*

Proof. To prove the theorem we will establish consecutively that the transformation is injective and surjective.

We notice that every step on the square lattice has a unique for itself combination of two steps on the honeycomb lattice. Something more – unique two points from the walk on the hexagonal grid, which are divided by two steps. Hence, one walk on the square grid determines in a unique manner the first, second, third, fourth, and so on, till the $2k+1^{st}$ point of the walk on the hexagonal grid (let us call this points odd and respectively the others – even). In fact, the whole hexagonal grid can be divided into points, which always will be even and others which are always odd (Fig. 10). Hence, two different walks on the square lattice determine, for the walks they are transformed into, different odd points. From here it follows that the transformation is injective.

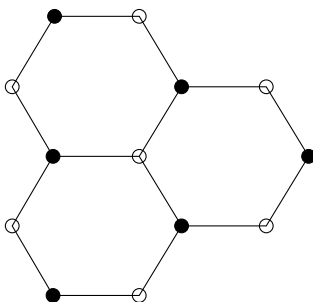


Fig. 10. Black points, which are odd, and white points, which are even

Now, let us start with the proof that the transformation is surjective. We will prove that every SSAW of $2n$ -steps is a result of the transformation of a SAW on the square lattice.

We consider the odd points of this walk and we notice that through every point there, the walk has passed exactly one time, because the only permitted intersection is in an even point. Moreover, every two odd points, through which the walk passes consecutively, correspond to the move on the square grid. This follows from the SSAW' characteristics. Thus we finished our proof. \square

We denote the number of SSAWs with length n by S_n . Theorem 4.2 implies that

$$S_{2n} = c_n,$$

$$\mu_{\mathbb{Z} \times \mathbb{Z}} = \left(\lim_{n \rightarrow \infty} \sqrt[n]{S_n} \right)^2$$

as we know that $\lim_{n \rightarrow \infty} \sqrt[n]{S_n}$ exists, because of Fekete's lemma.

Let us call *branches* the parts where the walk self-intersects and passes two times through one of the hexagon's sides, while the other part of the walk will be named the *main branch* (Fig. 11). The main branch is simply a SAW on the hexagonal lattice and determines, in a unique manner, where the branches will be attached.

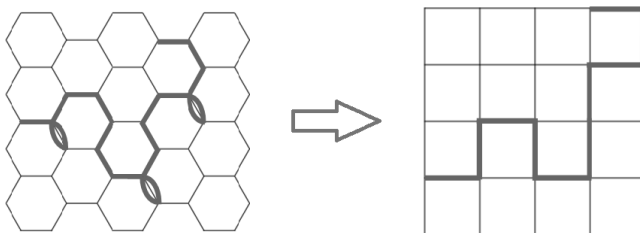


Fig. 11. An SSAW with three branches and length of the main branch equal to 14 is transformed into a SAW on the square lattice with length 10

If we want to find c_n , we need to know the number of SSAWs with a length of the main branch $n - k$ and $\frac{k}{2}$ branches, for all possible k . A branch appears whenever on the square lattice we make a right step followed by a step upwards or whenever we have a step downwards followed by a step to the left. We call these turns – *branch-creating* (Fig. 12).

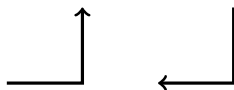


Fig. 12. Branch-creating turns

Let A_n be the number of turns all c_n SAWs on the square lattice make. Then the number of branch-creating turns is $\frac{A_n}{4}$. On average a SAW on the square lattice makes $\frac{A_n}{4c_n}$ branch-creating turns. We take the first 22 values of A_n from [PR] and moreover calculate it up to $n = 27$. Then we examine the fraction

$$\frac{A_n}{c_n} = x_n$$

for all n smaller than 28 (Fig. 13). A table is shown in Appendix C.

Conjecture 4.3. *For sufficiently large n , on average, the number of turns a SAW of length n on the square lattice makes is*

$$x_n \approx \frac{3}{5}n.$$

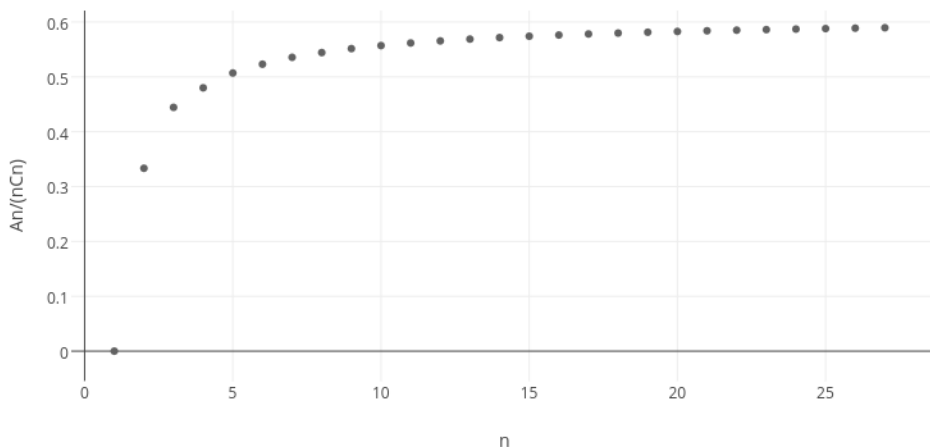


Fig. 13. Number of turns on average divided by n , as n grows

On average the length of the main branch will be $2n - \frac{x_n}{2}$, because every branch is made out of 2 steps. Let us, for example, accept that $\lim_{n \rightarrow \infty} \frac{x_n}{n} = 0.6$. Then $\lim_{n \rightarrow \infty} \frac{2n - \frac{x_n}{2}}{n} = \frac{17}{10}$. Denote the number of SAWs on the hexagonal lattice of length n with h_n . Let us consider the values of n when it is divisible by 10 ($n = 10k$). Let $x_1, x_2, \dots, x_{c_{10k}}$ be the lengths of the main branches of all c_{10k} transformed SAWs from the square lattice of length n . Therefore we have:

$$\lim_{k \rightarrow \infty} \frac{x_1 + x_2 + \dots + x_{c_{10k}}}{kc_{10k}} = \lim_{k \rightarrow \infty} \frac{17kh_{17k}}{kh_{17k}}.$$

The purpose of this result is to be able to obtain a purely mathematical close bound for the number of walks and for the connective constant without the work of thousands of hours of computer computations. If we manage to prove that

$$(3) \quad x_1 + x_2 + \dots + x_{c_{10k}} \leq 17kh_{17k}$$

for sufficiently large k . Then we will have that

$$\lim_{k \rightarrow \infty} \frac{c_{10k}}{h_{17k}} \leq 1.$$

Hence, for sufficiently large n we have that

$$c_{10k} \leq h_{17k}.$$

Moreover, this yields

$$\begin{aligned} \lim_{n \rightarrow \infty} \sqrt[10k]{c_{10k}} &\leq \lim_{n \rightarrow \infty} \sqrt[10k]{h_{17k}}, \\ \mu_{\mathbb{Z} \times \mathbb{Z}} &\leq \mu_H^{\frac{17}{10}} \approx 2.84. \end{aligned}$$

However, one should notice that the bound for the connective constant follows directly from the inequality (3) and does not need our previous computations. In addition, proving a lower bound for x_n would again yield an upper bound, however, they will be weaker.

Consider a SAW on the hexagonal lattice which does not move in a direction which is partially south. Then it can be seen that the number of SAWs of this type of length n is F_{n+1} where F_i is the i^{th} Fibonacci number (F_0 and F_1 equal 1). Could we compare these SAWs and SSAWs in some way? Let us assume that

$$F_n \leq S_n.$$

Therefore

$$\begin{aligned} \frac{1 + \sqrt{5}}{2} &\leq \lim_{n \rightarrow \infty} \sqrt[n]{S_n}, \\ \left(\frac{1 + \sqrt{5}}{2}\right)^2 &\approx 2,618 \leq \mu_{\mathbb{Z} \times \mathbb{Z}}. \end{aligned}$$

We hope that in the future we will be able to prove that

$$\begin{aligned} F_n \leq c_n, \quad c_{10k} &\leq h_{17k}, \\ 2.618 &\leq \mu_{\mathbb{Z} \times \mathbb{Z}} \leq 2.84. \end{aligned}$$

Moreover, we want to prove the above inequalities without any or with little computer computations as the value of μ_H was obtained purely mathematically. We presented a way in which this might happen. For comparison, the best known bounds nowadays (see [8]) are:

$$\begin{aligned} 2.62002 &\leq \mu_{\mathbb{Z} \times \mathbb{Z}} \leq 2.67919, \\ \mu^n &\leq c_n \leq \mu_{\mathbb{Z} \times \mathbb{Z}}^n e^{k\sqrt{n}}. \end{aligned}$$

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Appendix A. Upper bound for $\mu_{[-1,2]}$. We consider the other 3 types of irreducible bridges. We use the same method to make an injective transformation that maps the irreducible bridges to SAWs on a lattice strip of width one. Then, after finding the generating function of the codomain, we decrease some of the coefficients. The calculations are in Table 3.

Table 3

	O_O	I_O	O_I	I_I
Transformed SAWs	$\frac{t^2}{1 - 2t + t^2 - t^4}$	$\frac{(1 - t)t}{1 - 2t + t^2 - t^4}$	$\frac{(1 - t)t}{1 - 2t + t^2 - t^4}$	$\frac{t^2}{1 - 2t + t^2 - t^4}$
Extracting the added steps	$\frac{1}{1 - 2t + t^2 - t^4}$	$\frac{(1 - t)}{1 - 2t + t^2 - t^4}$	$\frac{(1 - t)}{1 - 2t + t^2 - t^4}$	$\frac{t^2}{1 - 2t + t^2 - t^4}$
Decreasing the coefficients with ...	$1 + 2t + 3t^2 + 4t^3 + 5t^4 + 10t^5 + 17t^6 + 24t^7 + 45t^8 + 72t^9 + 109t^{10} + 188t^{11} + 301t^{12} + 474t^{13}$	$1 + t + 2t^4 + 4t^5 + 6t^6 + 11t^7 + 16t^8 + 26t^9 + 44t^{10} + 67t^{11} + 115t^{12} + 180t^{13}$	$1 + t + 2t^4 + 4t^5 + 6t^6 + 11t^7 + 16t^8 + 26t^9 + 44t^{10} + 67t^{11} + 115t^{12} + 180t^{13}$	$2t^3 + 3t^4 + 4t^5 + 6t^6 + 10t^7 + 17t^8 + 28t^9 + 45t^{10} + 72t^{11} + 115t^{12} + 186t^{13}$

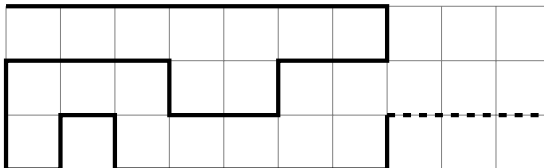


Fig. 15. Fig. 7 after the transformation to an irreducible bridge of type I_O , that moves in the “opposite” direction

Appendix B. Lower and upper bounds for the number of SAWs on the $\mathbb{Z} \times \{-1, 0, 1\}$ and $\mathbb{Z} \times \{-1, 0, 1, 2\}$ lattices. We use the Hammersley Welsh-Method which was used to find bounds for the number of SAWs on the $\mathbb{Z} \times \mathbb{Z}$ lattice (see [8, p. 57]).

B.1. Lower bound. We introduce Fekete’s lemma.

Lemma B.1. For every subadditive set $\{a_n\}_{n=1}^\infty$, the bound $\lim_{n \rightarrow \infty} \frac{a_n}{n}$ exists and is equal to $\inf \frac{a_n}{n}$.

Let y be equal to 1 or 2. Then

$$c_{[-1,y]n+m} \leq c_{[-1,y]n}c_{[-1,y]m}$$

$$\log c_{[-1,y]n+m} \leq \log c_{[-1,y]n} + \log c_{[-1,y]m}.$$

Therefore,

$$\inf \frac{\log c_{[-1,y]n}}{n} = \lim_{n \rightarrow \infty} \frac{\log c_{[-1,y]n}}{n}$$

$$\log \mu_{[-1,y]} = \inf \frac{\log c_{[-1,y]n}}{n}$$

$$\mu_{[-1,y]}^n \leq c_{[-1,y]n}$$

for $n \geq 1$.

B.2. Upper bound. We will prove (1) (Section 2) for the $\mathbb{Z} \times \{-1, 0, 1\}$ lattice, however, one can prove (2) (Section 3) for the $\mathbb{Z} \times \{-1, 0, 1, 2\}$ lattice in the same way.

B.2.1. $\mathbb{Z} \times \{-1, 0, 1\}$ lattice. Before going into details, we need several definitions and one lemma.

Definition B.2. An n -step half-space walk (all points after the first one are on the right of the line, parallel to the x -axis passing through it) is a SAW, whose x -axis coordinates of the points satisfy the following inequality:

$$x_0 < x_i$$

for all $i = 1, 2, \dots, n$.

The number of n -step half-space walks is denoted with $h_{[-1,1]n}$. By convention, $h_{[-1,1]0} = 1$.

In particular, every bridge is a half-space walk.

Definition B.3. The span of a n -step SAW is the difference between the smallest and biggest x -axis coordinate of points, which are part of the walk:

$$\max_{0 \leq i \leq n} x_i - \min_{0 \leq i \leq n} x_i.$$

The number of n -step half-space walks (respectively bridges) starting at the origin $(0, 0)$ and having span A is denoted by $h_{[-1,1]n,A}$ (respectively $b_{[-1,1]n,A}$).

Note that $h_{[-1,1]n,0}$ is 1 if $n = 0$, and it is 0 otherwise.

Lemma B.4. For each integer $A > 0$, let $P_F(A)$ denote the number of partitions of A into distinct integers, whose number is less than 4 (i.e the number of ways to write $A = A_1 + \dots + A_k$, where $A_1 > \dots > A_k > 0$ and $k \leq 3$). Then

$$P_F(A) \leq 1 + A + A^2.$$

By assumption we let $P_F(0) = 1$ since $1 \leq 1 + 0 + 0$.

Proof. If $k = 1$, then we have one way. If $k = 2$, then we have at most A ways, as for every choice for A_1 , we have at most one possibility for A_2 . The next case is analogical, as for $k = 3$ we count all possibilities for A_1 and A_2 , and we get at most A^2 different sums. \square

The following proposition contains the first part of the proof of our upper bound.

Proposition B.5. For every $n \geq 0$,

$$h_{[-1,1]n} \leq P_F(n)b_{[-1,1]n}.$$

Proof. Let us have an n -step half-space walk denoted by w that starts at the origin $(0, 0)$. Let $n_0 = 0$. For each $i = 1, 2, \dots$, respectively define $A_j(w)$ and $n_j(w)$ so that

$$A_i = \max_{n_{i-1} \leq j \leq n} (-1)^i (x_{n_{i-1}} - x_j)$$

and n_i is the largest value of j , for which this maximum is attained. The recursion is stopped at the smallest integer k such that $n_k = n$; this means that $A_{k+1}(w)$ and $n_{k+1}(w)$ are not defined. Observe that $A_1(w)$ is the span of w ; in general A_{i+1} is the span of the SAW (w_{n_i}, \dots, w_n) (w_i is the $i + 1$ point of the walk w), which is either a half-space walk or the reflection of one. Moreover, each of the subwalks $(w_{n_i}, \dots, w_{n_{i+1}})$ is either a bridge or the reflection of one. Also observe that $A_1 > A_2 > \dots > A_k > 0$ and that as we are working on the grid $\mathbb{Z} \times \{-1, 0, 1\}$, then $k \leq 3$, because when we reach w_{n_1} , the rest of the walk cannot have points on at least one of the lines. This follows from the fact that the last

rightmost point is higher or lower (let us assume that it is lower) from the first rightmost point, and all other points need to have a smaller x -axis coordinate. As a result, since we have a half-space walk, all the points need to be below the walk with ends (w_{n_0}, w_{n_1}) . From here we can see that the statement is true. As the same process continues, we find that $k \leq 3$.

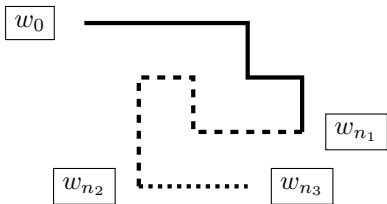


Fig. 16. A half-space walk w in $H_{14}[4, 3, 2]$

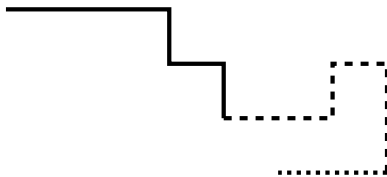


Fig. 17. The transformed walk w' in $H_{14}[7, 2]$

For every decreasing sequence of k positive integers $a_1 > a_2 > \dots > a_k > 0$, let $H_n[a_1, a_2, \dots, a_k]$ be the set of n -step half-space walks w with $w_0 = (0, 0)$ and $A_1(w) = a_1, \dots, A_k(w) = a_k$ and $n_k(w) = n$. Note that in particular $H_n[a]$ is the set of n -step bridges of span a .

Given an n -step half-space walk w , define a new n -step walk w' as follows: for $0 \leq j \leq n_1(w)$, define $w'_j = w_j$; and for $n_1(w) < j \leq n$, define w'_j to be the reflection of the point w_j in the hyperplane $x_1 = A_1(w)$. Observe that if w is in $H_n[a_1, a_2, \dots, a_k]$, then w' is in $H_n[a_1 + a_1, a_3, \dots, a_k]$; moreover, this transformation maps an unique walk (the transformation is one-to-one), so

$$|H_n[a_1, a_2, \dots, a_k]| \leq |H_n[a_1 + a_2, a_3, \dots, a_k]|.$$

Therefore, summing over all possible sequences $a_1 > \dots > a_k > 0$, we get that

$$\begin{aligned} h_{[-1,1]n} &= \sum |H_n[a_1, \dots, a_k]| \leq \sum |H_n[a_1 + \dots + a_k]| \\ &= \sum b_{[-1,1]n, a_1 + \dots + a_k} \end{aligned}$$

which tells us that

$$h_{[-1,1]n} \leq \sum P_F(A) b_{[-1,1]n, A}.$$

Note that $P_F(A) \leq P_F(n)$ for $A \leq n$. Hence,

$$h_{[-1,1]n} \leq P_F(n) \sum_{A=1}^n b_{[-1,1]n,A} = P_F(n)b_{[-1,1]n}$$

which proves the proposition. \square

Therefore, we are ready to prove our upper bound.

Proof. Given an arbitrary n -step SAW w , let $M = \min x_j$ and m be the largest j such that $x_j = M$. Then (w_m, \dots, w_n) is a half-space walk, as is

$$(w(m) - (1, 0), w(m), w(m - 1), \dots, w(0)).$$

Using this decomposition method, as well as Proposition B.5 and the inequality $b_{[-1,1]i}b_{[-1,1]j} \leq b_{[-1,1]i+j}$ (which follows from the fact that whenever we concatenate two bridges we get a new bridge) we obtain:

$$\begin{aligned} c_{[-1,1]n} &\leq \sum_{m=0}^n h_{[-1,1]n-m}h_{[-1,1]m+1} \leq \sum_{m=0}^n b_{[-1,1]n-m}b_{[-1,1]m+1}P_F(m+1)P_F(n-m) \\ &\leq b_{[-1,1]n+1} \sum_{m=0}^n (1 + (m + 1) + (m + 1)^2)(1 + (n - m) + (n - m)^2) \\ &\leq b_{[-1,1]n+1}((n + 1) + 2(n + 1)^2 + 3(n + 1)^3 + 2(n + 1)^4 + (n + 1)^5) \end{aligned}$$

for all n . Therefore, since $b_{[-1,1];n+1} \leq \mu_{[-1,1]}^{n+1}$ (the proof of this fact, as for our lower bound for the number of SAWs, uses Fekete’s lemma, when concerning superadditive sequences), we have

$$c_{[-1,1]n} \leq \mu_{[-1,1]}^{n+1}((n + 1) + 2(n + 1)^2 + 3(n + 1)^3 + 2(n + 1)^4 + (n + 1)^5). \quad \square$$

Corollary B.6. *For all $n \geq 2$ we have that*

$$\frac{\mu_{[-1,1]}^{n-1}}{(n + 1) + 2(n + 1)^2 + 3(n + 1)^3 + 2(n + 1)^4 + (n + 1)^5} \leq b_{[-1,1]n} \leq \mu_{[-1,1]}^n.$$

Proof. The left bound follows from (1) and from the fact that $\mu_{[-1,1]}^n \leq c_{[-1,1]n}$. The right bound can be proven by using the superadditive sequence $\{\log b_{[-1,1]n}\}_{n=1}^\infty$. Thus, $\lim_{n \rightarrow \infty} \sqrt[n]{b_{[-1,1]n}} = \mu_{[-1,1]}$. \square

B.2.2. $\mathbb{Z} \times \{-1, 0, 1, 2\}$ lattice. When using the method for the $\mathbb{Z} \times \{-1, 0, 1, 2\}$ lattice we would have that $P_F(A) \leq 1 + A + A^2 + A^3$. Hence, we would have that

$$\begin{aligned} c_{[-1,2]n} &\leq \sum_{m=0}^n h_{[-1,2]n-m}h_{[-1,2]m+1} \leq \sum_{m=0}^n b_{[-1,2]n-m}b_{[-1,2]m+1}P_F(m+1)P_F(n-m) \\ &\leq b_{[-1,2]n+1} \sum_{m=0}^n (1 + (m + 1) + (m + 1)^2 + (m + 1)^3)(1 + (n - m) + (n - m)^2 + (n - m)^3) \end{aligned}$$

$\leq b_{[-1,2]_{n+1}}((n+1)+2(n+1)^2+3(n+1)^3+4(n+1)^4+3(n+1)^5+2(n+1)^6+(n+1)^7)$
 for all $n \geq 1$. Thus, since $b_{[-1,2]_{n+1}} \leq \mu_{[-1,2]}^{n+1}$ (the proof again uses Fekete's lemma),
 we have

$$c_{[-1,2]_n} \leq \mu_{[-1,2]}^{n+1}((n+1) + 2(n+1)^2 + 3(n+1)^3 + 4(n+1)^4 + 3(n+1)^5 + 2(n+1)^6 + (n+1)^7).$$

We have the analogous corollary that

$$\lim_{n \rightarrow \infty} \sqrt[n]{b_{[-1,2]_n}} = \mu_{[-1,2]}.$$

Appendix C. Number of turns on the square lattice.

Table 5

n	c_n	A_n	$\frac{A_n}{c_n} = x_n$	$\frac{x_n}{n}$
1	4	0	0	0
2	12	8	0.666666667	0.333333333
3	36	48	1.333333333	0.444444444
4	100	192	1.92	0.48
5	284	720	2.535211268	0.507042254
6	780	2448	3.138461538	0.523076923
7	2172	8144	3.749539595	0.535648514
8	5916	25760	4.354293442	0.54428668
9	16268	80752	4.963855422	0.551539491
10	44100	245648	5.570249433	0.557024943
11	120292	743312	6.179230539	0.561748231
12	324932	2205168	6.786552263	0.565546022
13	881500	6518864	7.395194555	0.56886112
14	2374444	19003088	8.003173796	0.571655271
15	6416596	55258640	8.611830946	0.574122063
16	17245332	159004448	9.220144211	0.576259013
17	46466676	456716656	9.828907409	0.578171024
18	124658732	1301118688	10.43744523	0.579858068
19	335116620	3701802736	11.04631199	0.581384841
20	897697164	10462677056	11.6550185	0.582750925
21	2408806028	29541536240	12.26397472	0.583998796
22	6444560484	82959601504	12.87280982	0.585127719
23	17266613812	232785788080	13.48184367	0.586167116
24	46146397316	650238685680	14.09077899	0.587115791
25	123481354908	1815160933616	14.69987866	0.587995146
26	329712786220	5047538209296	15.30889435	0.588803629
27	881317491628	14028855411952	15.91804945	0.589557387