SOME OBSERVATIONS ON SELF-AVOIDING WALKS

by

Yenisi Das

under the guidance of

Prof. Siva Athreya

Project Report

S.N. Bhatt Memorial Excellence Fellowship Program

ICTS, Bengaluru

July 2023

Contents

1 Introduction

Self-avoiding walks have been extensively studied and analyzed in the scientific community due to their significant applications in the fields of physics, chemistry, and biology. They are an important model for describing the behavior of polymer chains, and protein folding, and are used in DNA conformational analysis [10] all of which have a similar characteristic of not allowing self-intersections. The main reference for this project is [8]. Further details can be found in [13], [4], [14], and [9].

We begin by getting an intuitive idea of what a self-avoiding walk is through a simple example. Suppose you are at Vidyarthi Bhavan and you want to go to the Lalbagh Metro Station. While walking, you follow a rule that you must not revisit any intersection you have already passed through. You continue walking and turning at intersections until you have reached the metro station. If you reach the metro station in n steps, we will say that you have created a self-avoiding walk of length n from Vidyarthi Bhavan to the Lalbagh Metro Station.

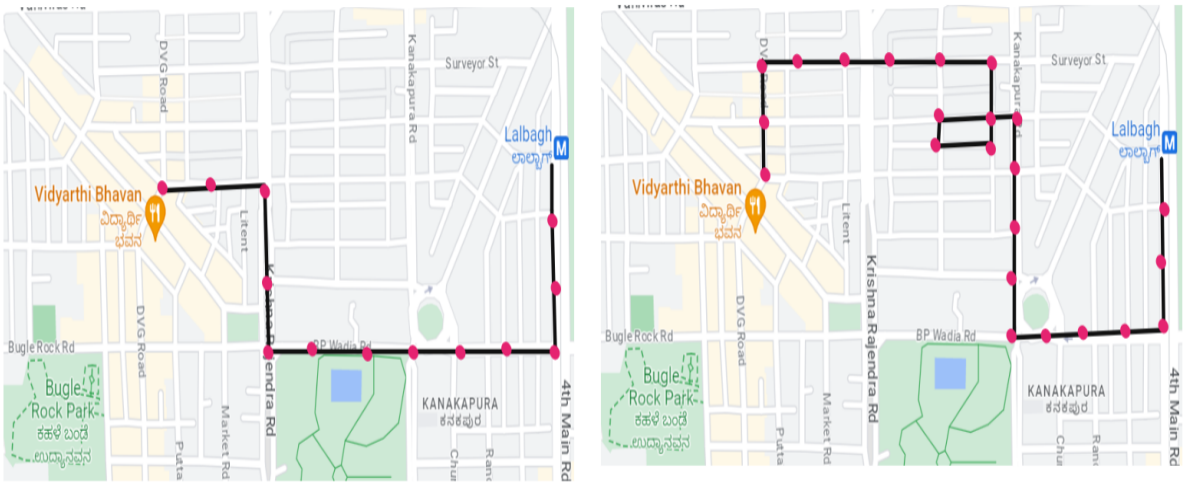

Figure 1: A self-avoiding walk (left) and a walk with intersections (right) to the metro station

The growing self-avoiding walk (GSAW) is constructed sequentially by looking at the available directions (unoccupied) at each step and choosing any one of them according to some preset probabilities $p_0, ..., p_m$ where m is the number of available directions to move into. Note that we can get trapped while doing this if there are no available directions to move into. Thus, a growing self-avoiding walk is of varying length.

In this report, we focus on the following questions:

1. How many self-avoiding walks are there of length n, for large n?
2. Given n, how can we sample a self-avoiding walk of length n uniformly?
3. On average, what is the length of a growing self-avoiding walk before it gets trapped?

We begin a discussion on how self-avoiding walks are used as models in statistical physics and chemistry.

1.1 Motivation and Literature

Self-avoiding walks have emerged as a powerful tool for modeling the behavior of polymer chains. A polymer is composed of numerous 'monomers', or groups of atoms, linked by chemical bonds. The functionality of a monomer refers to the number of chemical bonds available, indicating the number of monomers it must bond with. If each monomer has functionality two, it results in a linear polymer.

Linear polymers can be enormous, comprising over 10^5 monomers, making the length scale of the entire polymer macroscopic, A linear polymer consisting of $N+1$ monomers can be labeled from one end to the other as $0, 1, \ldots, N$. The location of the i^{th} monomer can be denoted by $x(i) \in \mathbb{R}^3$, with the i^{th} bond represented by the line segment joining $x(i-1)$ to $x(i)$. Usually, the length of each bond is roughly constant throughout the chain, along with the angle between each consecutive monomer-monomer bond.

A possible model for the spatial configuration of a linear polymer is a random walk in $\mathbb{Z}^3$, known as the ideal polymer chain. The random walk approximation for polymers was proposed around 80 years ago by a German chemist called Kuhn [7] and a Hungarian physicist Guth [2] independently. Years after this assumption was proven incorrect. A new answer to the questions about this model was discovered by the Nobel laureate Flory [1] and Orr [11] who suggested that while the random walk tends to trap themselves, the monomers try to bounce away from each other. The ideal polymer chain had a fundamental limitation, namely the excluded volume effect.

The presence of a monomer at position x prohibits any other part of the polymer from getting too close to x, meaning that other monomers are excluded from a certain volume of space. This is the excluded volume effect. Taking this effect into account reveals that a self-avoiding walk is a more suitable model for a linear polymer than a random walk. The self-avoiding walk model is ideal for the case of a dilute polymer solution, where the polymers are far apart, leading to little interaction between distinct molecules, and a good solvent minimizes attractive forces between monomers.

Polymer scientists are interested in understanding the behavior of the set of self-avoiding walks as the number of monomers grows toward infinity. While real polymers exist in continuous space, it turns out that the behavior of self-avoiding walks on a lattice is a good approximation for large polymers, and studying this simpler mathematical model can give valuable insights into the properties of real polymers.

The rest of the article is organized as follows. In section 2 we count the number of SAWs and see that itgrows exponentially. In the next section, we describe a Monte-Carlo method by which a markov chain on the state space of all self-avoiding walks of a given length samples a self-avoiding walk uniformly. The algorithm is known as the pivot algorithm. Then in section 4 we discuss one of the models to sequentially generate self-avoiding walks and discuss the phase transition. We also discuss the mean length before such a walk gets trapped for different values of β which a function

of temperature associated with the model.

2 Counting Self-Avoiding Walks

Let $\mathbb{Z}^d$ be the integer lattice. We begin by defining the self-avoiding walk of length n:

Definition 2.1. *An n-step self-avoiding walk can be defined as a function $\omega : \{0, 1, ..., n\} \to \mathbb{Z}^d$, beginning at the site x, i.e. $\omega(0) = x$, satisfying*

$$|\omega(j+1) - \omega(j)| = 1, \textit{and} \;\; \omega(i) \neq \omega(j) \; \forall \; i \neq j$$

.

We write $|\omega| = n$ to denote the length of ω, and we denote the components of $\omega(j)$ by $\omega_i(j)$ where $i = 1, ..., d$. Let C_n denote the number of N -step self-avoiding walks beginning at the origin. By convention, $C_0 = 1$.

We now show some elementary bounds of C_n in order to understand how it grows. Let us fix d. Consider the set of self-avoiding walks in the d-dimensional integer lattice space which, for each axis, only take steps in positive directions. These are all obviously self-avoiding, and at each point, there are d possible choices of directions, so there are d^n such self-avoiding walks. Thus,

$$C_n \geq d^n.$$

Now consider all walks of length n that never return to the site they were at in the previous step, that is, the set of all walks for which $\omega(j-1) \neq \omega(j+1)$ for $j = 1, ..., n-1$ Then at each site after the initial one, there are $2d-1$ possible choices, and therefore there are $2d(2d-1)^{n-1}$ such walks. All self-avoiding walks have this property, so there are at most $2d(2d-1)^{n-1}$ self-avoiding walks.

Therefore we have shown that

$$d^n \leq C_n \leq 2d(2d-1)^{n-1}.$$

It seems that C_n grows exponentially in n. We make the following intuitive observation about the concatenation of two SAWs for showing that C_n grows exponentially. Every self-avoiding walk of length $n+m$ may be split into two smaller self-avoiding walks; one of length n and one of length m but the concatenations of every n and m length walk is not self-avoiding as seen in the pictures below.

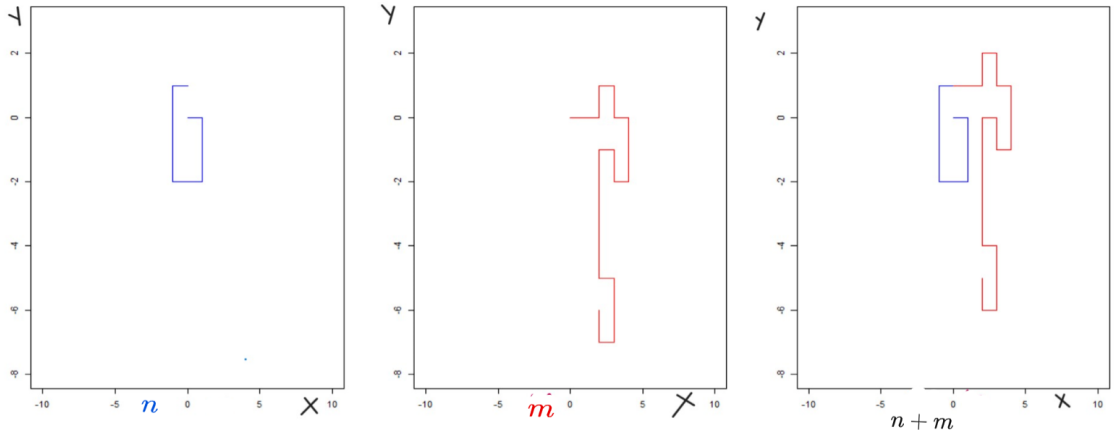

Figure 2: Concatenation of a SAW of length 10 to a SAW of length 20 creating a SAW of length 30

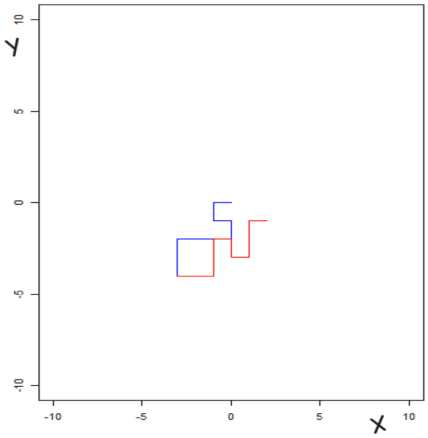

Figure 3: Concatenation of a SAW of length 10 to a SAW of length 10 resulting in intersections

We make the above observation precise in the proposition below.

Proposition 2.2. $C_{n+m} \leq C_m C_n$.

Proof of Proposition 2.2. : Let S_{n+m}, S_n, and S_m be the set of self-avoiding walks of length $n+m, n$, and m respectively. Consider the function $f : S_{n+m} \to (S_n \times S_m)$ defined by $f(\omega) = (\omega^{(1)}, \omega^{(2)})$ where $\omega \in S_{n+m}, \omega^{(1)} \in S_n$, $\omega^{(2)} \in S_m$

$$\text{and } \omega^{(1)} : \{0, 1, ..., N\} \to \mathbb{Z}^d, \omega^{(1)}(k) = \omega(k), k = 0, 1, ..., n$$

,

$$\omega^{(2)} : \{0, 1, ..., M\} \to \mathbb{Z}^d, \omega^{(2)}(0) = 0$$

.

$$\omega^{(2)}(k) = \omega(k+n) - \omega(n), k = 0, 1, ..., m$$

. It is clear that f is injective. Therefore $C_{n+m} = |S_{n+m}| \leq |S_n||S_m| = C_n C_m$. $\square$

We are now ready to state our first result. We show that indeed the number of self-avoiding walks of length n grows exponentially in n.

Theorem 2.3. *:*

$$\lim_{n\to\infty} C_n{}^{\frac{1}{n}} = \mu$$

The key idea used to prove Theorem 2.3 is the subadditivity of the self-avoiding walks. We shall prove this in section 5.1. The limit μ was first shown to exist by Hammersly and Morton [3]. Roughly, C_n is of order μ^n for large n, so μ is the average number of possible next steps for a long self-avoiding walk. A list of estimated values of μ for some lattices from [6] and [13] are given below:

Lattice	μ
$\mathbb{Z}^2$	2.638
$\mathbb{Z}^3$	4.683
$\mathbb{Z}^4$	6.772
$\mathbb{Z}^5$	8.838
$\mathbb{Z}^6$	10.878

3 Uniformly sampling a self-avoiding walk of length n

We now proceed to answer the second question by using the Monte-Carlo method to sample a self-avoiding walk of length n uniformly. The idea is to construct a Markovov chain on the state space of all self-avoiding walks (SAWs) of a given length. The algorithm we use to do this is called the pivot algorithm. As the algorithm progresses, the Markov chain approaches a stationary distribution. In the case of the pivot algorithm, this stationary distribution corresponds to the uniform distribution of SAWs of the given length. Convergence to the stationary distribution ensures that the algorithm generates SAWs uniformly at random.

We now see how the pivot algorithm is implemented.

3.1 The Pivot Algorithm

The idea behind the pivot algorithm is to start with a self-avoiding walk and then make small perturbations to its shape by rotating segments and reflecting segments around pivot points and accepting if the resulting path remains self-avoiding and rejecting the walk if it has intersections.

1. First, a self-avoiding walk is created by generating an ordinary random walk, where if it intersects itself, we start over and continue until we have an N-step SAW.

2. A pivot point k along the walk ($0 \leq k \leq N-1$) is chosen according to any preset strictly positive probabilities $p_0, ..., p_{N-1}$.

3. Let G be the group of orthogonal transformations (about the origin) that leave $\mathbb{Z}^d$ invariant. Then the symmetry operation $g \in G$ can be chosen according to any preset probability distribution $\{q_g\}_{\{}g \in G\}$ that satisfies $q_g = q_g^{-1}$ for all g, and has enough nonzero entries to ensure ergodicity. Now we apply this operation to the walk from the pivot point k onwards.

Elements of the group of orthogonal transformations An element $g \in G$ is a d by d orthogonal matrix with integer entries; so it suffices to specify the columns of g, which are $ge_1, ge_2, ..., ge_d$, where $e_1, e_2, ..., e_d$ are the unit vectors in $\mathbb{Z}^d$. Hence, an element $g \in G$ can be specified uniquely by giving a permutation π of $1, ..., d$ and numbers $\sigma_1, ..., \sigma_d = \pm 1$, and setting $ge_i = \sigma_i e_{\pi\{i\}}$. It follows that the cardinality of G is $2^d d!$ (each of $d\,\sigma_i's$ have 2 choices and d numbers have $d!$ permutations).

4. Now we check if our generated walk is still valid. If it is, then we find another self-avoiding walk. Otherwise, the initial walk is counted again in the sample.

We now state a theorem about the ergodicity of the pivot algorithm. The ergodicity of the pivot algorithm means that if we run the pivot algorithm for a long enough time, it will eventually generate all possible configurations of the walk, and each configuration will be generated with the same probability.

Theorem 3.1. *The pivot algorithm is ergodic for self-avoiding walks on $\mathbb{Z}^d$ provided that all axis reflections, and either all 90° rotations or all diagonal reflections are given nonzero probability. In fact, any N-step self-avoiding walk can be transformed into a straight rod by some sequence of 2N-1 or fewer such pivots.*

It is proved in section 5.2. Theorem 3.1 shows that we do not need 180° rotations if we have axis reflections. The reverse case is the following theorem; for simplicity, we consider only $d = 2$.

Theorem 3.2. *The pivot algorithm is ergodic for self-avoiding walks on $\mathbb{Z}^2$ provided that the 180° rotation, and either both 90° rotations or both diagonal reflections, are given nonzero probability.*

The above theorem essentially says that we do not need axis reflections as long as we have 180° rotations. It is proved in section 5.3. We now look at the implementation of the pivot algorithm to sample a SAW of length 500 uniformly in R.

3.2 Implementing the Algorithm

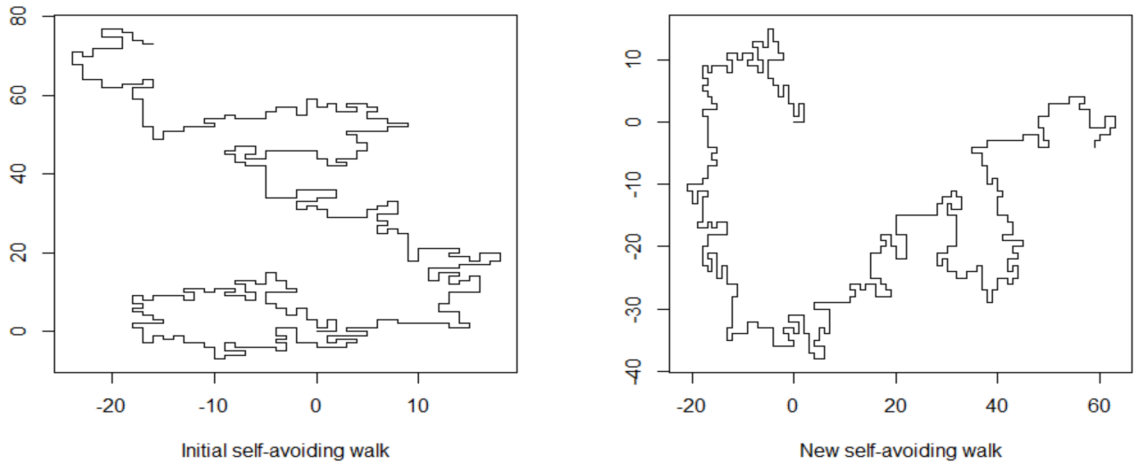

Figure 4: A self-avoiding walk of 500 steps generated uniformly

For implementing the algorithm to sample a SAW in 2 dimensions, we used the following three functions:

1. check.matrix.row(matrix, row): This function takes a matrix 'matrix' and a row 'row' as input and checks if any rows in the matrix are identical to the given row. It returns the index of the first row that matches or 0 if there are no matches. This is done to see if a site in a particular direction (given row) is occupied or not.

2. move(pos, orient): This function takes a position pos and an orientation orient as input and returns a new position that is shifted one unit in the given direction. The orientation can be 'U' (up), 'D' (down), 'R' (right), or 'L' (left). It is used while generating the initial SAW.

3. saw(steps): This function generates a self-avoiding random walk of steps 'steps'. It starts from the origin (0,0) and uses the move function to generate new positions. At each step, it checks which directions are available to move (i.e., not occupied by previous positions) and randomly chooses one of them. If no directions are available, it starts from the beginning.

We used the last two functions to generate the initial SAW. For the final SAW, I chose one pivot uniformly, i.e., $p_i = \frac{1}{n}, i = 0, ..., n-1$. Then we choose a symmetry operation uniformly, i.e., $q_i = \frac{1}{7}$ from the set of all symmetry operations $\{g_1, ..., g_7\}$ in dimension 2, where the symmetry operations are:

g_1: Rotation by $-\pi/2$

g_2: Rotation by $-\pi$. We have to change every up step to a down step and every left step to the right step and vice versa.

g_3: Rotation by $-\frac{3\pi}{2}$

g_4: Reflecting on the x-axis. By reflecting our walk on the x-axis we change every up step to a down step and every down step to an up step.

g_5: Reflecting on the y-axis. By reflecting our walk on the y-axis we change every left step to a right step and every right step to a left step.

g_6: Reflecting on the diagonal line $x = y$
g_7: Reflecting on the diagonal line $x = -y$

We multiplied the positions of the SAW from the pivot point onwards with the matrix corresponding to the chosen operation to reflect and rotate the self-avoiding walks. We chose multiple such pivot points and repeated the procedure to sample a SAW uniformly. The code in R will be available on request.

Now we move on to constructing a growing self-avoiding walk. In the next section, we delve into the topic of collapse transition. We explore the phase transition observed in self-avoiding walks on lattices where poor-solvent interactions are incorporated into the model.

4 Collapse transition

Here we discuss the growing self-avoiding walk and one of the many ways to construct such a walk. The main references for this section are [5] and [12].

4.1 Growing Self-Avoiding Walk

A growing self-avoiding walk (GSAW) on a lattice can be generated by taking a step in some direction from a lattice site, then a subsequent step to an open neighboring lattice site according to some probability distribution $p_1, ..., p_m$ (where m is the number of available steps), continuing to walk to any unoccupied site until no more sites are available. A growing SAW is thus sequentially generated and has varying lengths. We say a growing self-avoiding walk is trapped if there are no available sites. Consider the following model: If there are n available steps, then the probability of the i^{th} step is given by

$$p_i \propto e^{-\beta F_i}, \;\; i \in \{1, 2, ..., n\}$$

where

$$\beta = \frac{1}{T}, F_i = -m_i$$

and m_i is the number of non-adjacent nearest-neighbor occupied sites.

The number of non-adjacent nearest-neighbor occupied sites is explained below with the following example:

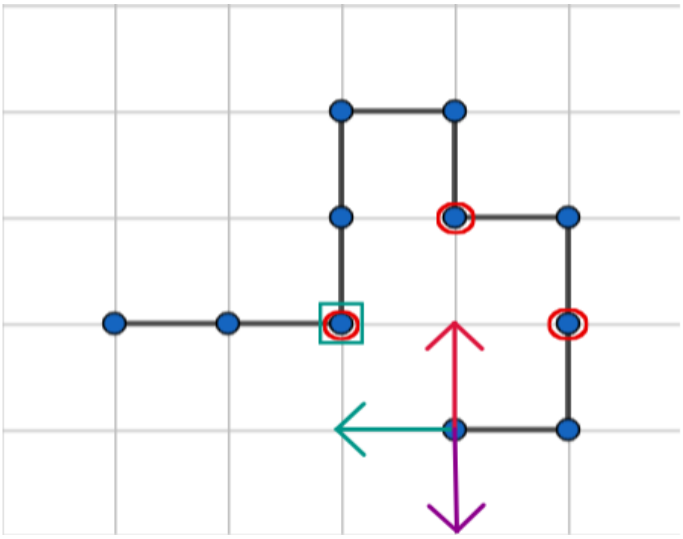

Figure 5: Non-adjacent nearest-neighbours

The number of non-adjacent nearest-neighbor occupied sites (m_i) for the step marked in red is 3 (marked in red circles). Thus the probability of taking the step marked in red is:

$$\text{P(Red step)} \propto e^{\frac{3}{T}}$$

The number of non-adjacent nearest-neighbor occupied sites (m_i) for the step marked in green is 1 (marked as a green square). Thus the probability of taking the step marked in green is:

$$\text{P(Green step)} \propto e^{\frac{1}{T}}$$

The number of non-adjacent nearest-neighbor occupied sites (m_i) for the step marked in purple is 0. Thus the probability of taking the step marked in purple is:

$$\text{P(Purple step)} \propto e^{\frac{0}{T}}$$

Note that the sum of these probabilities is 1, i.e.,

$$\frac{e^{\frac{3}{T}}}{1+e^{\frac{1}{T}}+e^{\frac{3}{T}}} + \frac{e^{\frac{3}{T}}}{1+e^{\frac{1}{T}}+e^{\frac{3}{T}}} + \frac{e^{\frac{3}{T}}}{1+e^{\frac{1}{T}}+e^{\frac{3}{T}}} = 1$$

When $\beta = 0$,

$$p_i = \frac{1}{\text{number of unoccupied sites}}$$

Thus, the probability of having an n-step walk is

$$\prod_{i=1}^{n} p_i$$

4.2 Phase Transition

Polymer chains interact with the solvent they are in. When it is in a good solvent, the excluded volume interactions between distant parts of the chain cause a polymer to adopt a "swollen coil" configuration that is larger than a noninteracting chain of the same length, described by the statistics of a self-avoiding walk. However, in a poor solvent, the effective attractive interactions between distant parts of the chain dominate over excluded volume interactions and the chain forms a compact "globule" that is smaller than an equivalent length noninteracting chain. As mentioned in [5], the coil-globule phase transition occurs in what is known as a "theta solvent," in which the attractive and repulsive interactions exactly cancel and the polymer can be described by the statistics of a random walk in three dimensions. An equivalent transition between swollen and collapsed states may be observed in self-avoiding random walks on lattices, where poor-solvent interactions are implemented in terms of an associated energy based on the number of nearest-neighbor contacts between non-adjacent sites on each walk.

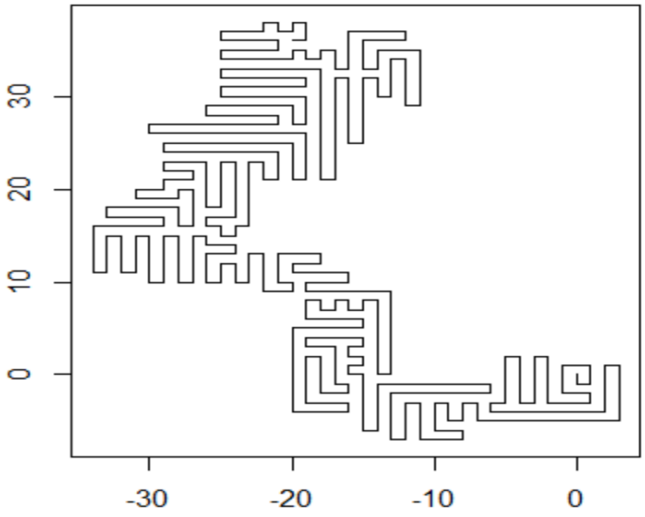

Figure 6: A SAW having attractive interactions

We study the trapping length of the growing SAWs in this model, that is, the length of the SAW before it gets trapped and has no available directions to go to. We do this by simulating growing SAWs and finding the mean trapping length.

For $\beta = 0$, we choose among the available steps uniformly. The mean trapping length from the simulations in R for $\beta = 0$ came out to be $70.648 \sim 71$ steps. We also study the mean trapping length for different values β. It seems from the plot that the mean trapping length increases with increasing values of β.

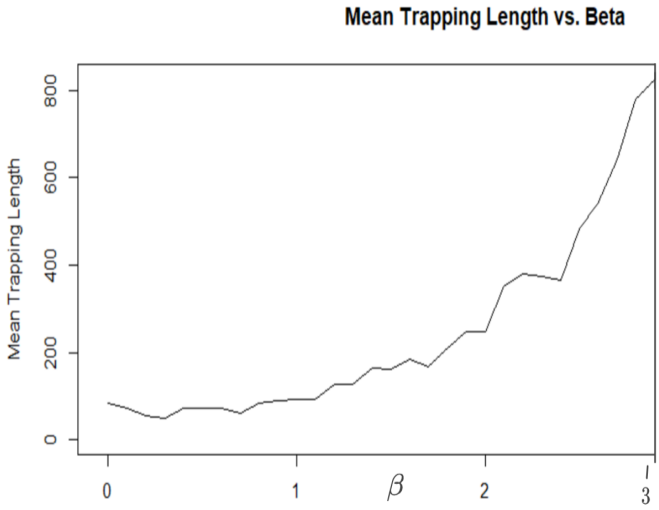

Figure 7: The mean trapping length vs. β

5 Proof of Theorems

5.1 Proof of Theorem 2.3

Here we show that C_n grows exponentially in n. Here is a plan of proof. Using the subadditivity property, in Claim 2.1, we establish that for $n = mq + r$ where n is the length of the walk and m is a fixed integer, $\frac{a_n}{n} \leq \frac{qa_m}{n} + \frac{a_r}{n}$. In Claims 2.2 and 2.3, we show that as $n \to \infty$, $\frac{qa_m}{n}$ goes to $\frac{a_m}{m}$ and $\frac{a_r}{n}$ goes to 0. Finally in Claim 3.7, we prove that the largest limit point of $\{\frac{a_n}{n}\}$ is less than or equal to the largest limit point of $\{\frac{qa_m}{n}\} + \{\frac{a_r}{n}\}$. Using these claims, we show that as $n \to \infty$, $\frac{a_n}{n}$ goes to $\inf\{\frac{a_m}{m} | m \geq 1\}$ which we call c.

Proof of Theorem 2.3. : Here we show that as n increases, the number of self-avoiding walks of length n grows exponentially. We prove this using the following four claims.

Claim 5.1. *:* $a_{kn} \leq ka_n$

Proof. : Fix n. Base case. For $k = 2, a_{2n} \leq 2a_n$ from (i)

Let the claim be true for $k = p$, i.e., $a_{pn} \leq pa_n$

Proof for $k = p + 1$: We know $a_{(p+1)n} = a_{pn+n} \leq a_{pn} + a_n$ Again $a_{pn} + a_n \leq pa_n + a_n = (p + 1)a_n$ Therefore, $a_{kn} \leq ka_n \; \forall \; k \geq 1$

Let $n = mq + r$ where m is a fixed integer and $0 \leq r \leq m - 1$ Now, $a_n = a_{mq+r} \leq a_{mq} + a_r \leq qa_m + a_r$, therefore,

$$\frac{a_n}{n} \leq \frac{qa_m}{n} + \frac{a_r}{n} \qquad -(1)$$

□

Claim 5.2. *: As $n \to \infty$,*

$$\frac{qa_m}{n} \to \frac{a_m}{m}$$

Proof. : Let $\epsilon > 0$ be given. To show: $|\frac{q}{n} - \frac{1}{m}| < \epsilon$ whenever $n \geq N$.

$$|\frac{q}{n} - \frac{1}{m}| = |\frac{n-r}{mn} - \frac{1}{m}| = |\frac{1}{m} - \frac{r}{mn} - \frac{1}{m}| = |\frac{r}{mn}| \leq \frac{1}{n} \quad since \quad \frac{r}{m} \leq 1$$

.

Now $\frac{1}{n} < \epsilon$ whenever $n \geq [\frac{1}{\epsilon}] + 1$.
So, we choose $N = [\frac{1}{\epsilon}] + 1$

□

Claim 5.3. *: As $n \to \infty$, $\frac{a_r}{n} \to 0$*

Proof. : We know $a_r \leq \max\{a_1, a_2, ..., a_{m-1}\} = k \quad \forall \quad n \geq 1$
To show: Let $\epsilon > 0$ be given. $|\frac{k}{n} - 0| < \epsilon$ whenever $n > N$. Choose $N = [\frac{k}{\epsilon}] + 1$.
Now, let

$$\alpha_n = \frac{a_n}{n}, \beta_{n,m} = \frac{qa_m}{n} + \frac{a_r}{n}$$

From (1), $\alpha_n \leq \beta_{n,m}$ We know from the previous 2 claims that

$$\lim_{n\to\infty} \beta_{n,m} = \frac{a_m}{m}$$

where $m \in \mathbb{N}$ is fixed.
Thus α_n and $\beta_{n,m}$ are bounded.

□

Limit point of a sequence: A real number p is said to be the limit point of a sequence $\{S_n\}_{n\geq 1}$ if for a given $\epsilon > 0, S_n \in (p - \epsilon, p + \epsilon)$ for infinitely many values of n.

We now prove 5 lemmas for the next part of the proof:

Lemma 5.4. *Fix m and let $n > m$. Let L be the largest limit point of $\{\beta_{n,m}\}$ Then for $\epsilon > 0$, there exists N such that $\{\beta_{n,m}\} \leq L + \epsilon \ \forall \ n \geq N$.*

Proof. Let there be infinitely many $\beta_{n,m}s$ above $L + \epsilon$. Then for every $m \in \mathbb{N}$ the sequence $\{\beta_{n,m}\}_{n>m}$ will have a $\beta_{n,m}$ such that $\beta_{n,m} \geq L + \epsilon$. Let x_i be the supremum of the $\{\beta_k\}_{k\geq i}$. Then $x_i \geq L + \epsilon \ \forall \ i$. But

$$L = \text{largest limit point of } \{\alpha_n\} = \lim_{n\to\infty} x_i \geq L + \epsilon$$

. We get a contradiction, so our assumption must be false. □

Lemma 5.5. *If $\alpha_n \leq M \ \forall \ n > N, N \in \mathbb{N}$, then the largest limit point of $\{\alpha_n\} \leq M$\$.*

Proof. Let M_1 be a limit point of $\alpha_n, M_1 \geq M$. Let $\epsilon = \frac{M_1 - M}{2}$. Since M_1 is a limit point of $\alpha_n, \exists\, N_1$ such that $M_1 - \epsilon \leq \alpha_n \leq M_1 + \epsilon \;\forall\; n \geq N_1$ i.e.

$$M_1 - \frac{(M_1 - M)}{2} \leq \alpha_n \leq M_1 + \frac{(M_1 - M)}{2} \;\forall\; n \geq N_1$$

$$\frac{M_1 + M}{2} \leq \alpha_n \leq \frac{3M_1 - M}{2} \;\forall\; n \geq N_1$$

Let $N_2 = \max(N_1, N)$. Then $\alpha_n \geq M \;\forall\; n > N_2$ and $\alpha_n \leq M \;\forall\; n > N_2$ is a contradiction. Therefore, the largest limit point of $\{\alpha_n\} \leq M$. □

Lemma 5.6. *Largest limit point of* $\{\alpha_n\} \leq$ *largest limit point of* $\{\beta_{n,m}\}$ *(*$m \in \mathbb{N}$ *is fixed and* $n > 1$*)*

Proof. Let the largest limit point of $\{\beta_{n,m}\}$ be L. By Lemma 5.4, there exists N such that $\beta_{n,m} \leq L + \epsilon \;\forall\; n \geq N$. Since $\alpha \leq \beta_{n,m}$ where m is fixed and $n \geq m$, there exists N such that

$$\alpha_n \leq L + \epsilon \;\forall\; n \geq N$$

. Therefore, only finitely many $\alpha_n s$ are above $L + \epsilon$. Using Lemma 5.5, this implies that the largest limit point of $\{\alpha_n\} \leq L + \epsilon$. Since $\epsilon \geq 0$ is arbitrary, the largest limit point of $\{\alpha_n\} \leq$ largest limit point of $\{\beta_{n,m}\}$ where m is fixed. □

Lemma 5.7. *If* $\{x_n\}$ *is a bounded and increasing sequence then* $\lim_{n\to\infty} x_n = \sup\{x_n : n \in \mathbb{N}\}$

Proof. Since $\{x_n\}$ is bounded, there exists a real number M such that $x_n \leq M \;\forall\; n \geq N$. Since $\{x_n\}$ is bounded above, $x^* = \sup\{x_n : n \in \mathbb{N}\} \in \mathbb{R}$. We will show that $x^* = \lim_{n\to\infty}\{x_n\}$. If $\epsilon \geq 0$ is given then $x^* - \epsilon$ is not an upper bound of the set $\{x_n : n \in \mathbb{N}\}$. Hence $\exists\, x_k$ such that $x^* - \epsilon < x_k$. $\{x_n\}$ is an increasing sequence implies that $x_k \leq x_n$ whenever $n \geq k$, so

$$x^* - \epsilon < x_k \leq x_n < x^* < x^* + \epsilon \;\forall\; n \geq k$$

. Therefore, we have $|x_n - x^*| \leq \epsilon \;\forall\; n \geq k$. Since $\epsilon \geq 0$ was arbitrary x_n converges to x^*.

□

Lemma 5.8.

$$\lim_{n\to\infty} \inf_{k\geq n}\{\frac{a_k}{k}\} = \sup_n \inf_{k\geq n}\{\frac{a_k}{k}\}$$

Proof. Define $M_n = \inf_{k\geq n}\{\frac{a_k}{k} : k \geq 1\}$. Now $M_n \leq M_{n+1}$, i.e., M_n is an increasing sequence. Since $\lim_{n\to\infty} M_n = \lim_{n\to\infty} \inf_{k\geq n}\{\frac{a_k}{k} : k \geq 1\}$. We also know that an increasing sequence which is bounded goes to $\sup_n \inf_{k\geq n}\{\frac{a_k}{k} : k \geq 1\}$ as $n \to \infty$. (By Lemma 5.7). Therefore,

$$\lim_{n\to\infty} \inf_{k\geq n}\{\frac{a_k}{k}\} = \sup_n \inf_{k\geq n}\{\frac{a_k}{k}\}$$

. □

Claim 5.9. *: Largest limit point of* $\{\alpha_n\} \leq \frac{a_m}{m}$ *for every* m.

Proof. We know that $\alpha_n \leq \beta_{n,m}$ for every $n \geq m$, where $m \in \mathbb{N}$ is fixed. By Lemma 3, the largest limit point of $\{\alpha_n\} \leq$ largest limit point of $\{\beta_{n,m}\}$. Since for $n \geq m$, where $m \in \mathbb{N}$ is fixed, we have $\alpha_n \leq \beta_{n,m}$ and $\lim_{n\to\infty} \beta_{n,m} = \frac{a_m}{m}$, so the largest limit point of $\{\alpha_n\} \leq \frac{a_m}{m}$. □

This implies that the largest limit point of $\{\alpha_n\} \leq \inf\{\frac{a_k}{k}, k \geq 1\}$

Claim 5.10. *Smallest limit point of* $\{\alpha_n\} \geq \inf\{\frac{a_k}{k}, k \geq 1\}$

Proof. We know, the smallest limit point of $\{\alpha_n\} = \lim_{n\to\infty} \inf_{k\geq n}\{\frac{a_k}{k}\}$. From the last lemma, we have $\lim_{n\to\infty} \inf_{k\geq n}\{\frac{a_k}{k}\} = \sup_n \inf_{k\geq n}\{\frac{a_k}{k}\}$ Therefore,

$$\sup_n \inf_{k\geq n}\{\frac{a_k}{k} : k \geq 1\} \geq \inf\{\frac{a_k}{k} : k \geq 1\}$$

. Therefore, the smallest limit point of $\{\alpha_n\} = \lim_{n\to\infty} \inf_{k\geq n}\{\frac{a_k}{k}\} = \sup_n \inf_{k\geq n}\{\frac{a_k}{k} : k \geq 1\} \geq \inf\{\frac{a_k}{k} : k \geq 1\}$. □

The largest limit point of $\{\alpha_n\} \leq \inf\{\frac{a_m}{m} | m \geq 1\}$

The smallest limit point of $\{\alpha_n\} \geq \inf\{\frac{a_m}{m} | m \geq 1\}$

From the above, the smallest limit point of $\{\alpha_n\} \geq$ largest limit point of $\{\alpha_n\}$.

Therefore, smallest limit point of $\{\alpha_n\}$ = largest limit point of $\{\alpha_n\}$ =$\inf\{\frac{a_m}{m} | m \geq 1\} = c$ (say)

Hence,

$$\lim_{n\to\infty} \frac{\log C_n}{n} = c$$

Thus, $\forall\ \epsilon > 0\ \exists\ N \in \mathbb{N}$ such that whenever $n \geq N, |\frac{\log C_n}{n} - c| < \epsilon$. Take $\epsilon = \frac{c}{2}$, then $\frac{c}{2} \leq \frac{\log C_n}{n} \leq \frac{3c}{2} \implies e^{\frac{nc}{2}} \leq C_n \leq e^{\frac{3nc}{2}}$. Therefore, $C_n \sim e^{nc}$. □

5.2 Proof of Theorem 3.1

We prove the ergodicity of the pivot algorithm. We first show that the pivot algorithm is irreducible. We set up some notation to prove this.

Notation: Let $\omega = (\omega(0), \omega(1), ..., \omega(N))$ be a self-avoiding walk of length N with $w(0)$ not necessarily equal to 0. Let $B(w)$ be the smallest rectangular box containing w. So, $B(w) = \{(x_1, ..., x_d) : m_i < x_i < M_i\}$ where $m_i = \min\{w_i(j), j = 0, 1, ..., N\}$ and $M_i = \max\{w_i(j), j = 0, 1, ..., N\}$ are the minimum and the maximum values of the i^{th} coordinate.

A face of $B(\omega)$ is any set of the form $\{x \in B(\omega) : x_i = m_i\}$ or $\{x \in B(\omega) : x_i = M_i\}$ for some $i = 1, 2, ..., d$.

Let $D(\omega) = \sum_{i=1}^{d} M_i - m_i$ and $A(\omega) = |\{i : 0 \leq i \leq N, \omega_i = \frac{1}{2}(\omega_{i-1} + \omega_{i+1})\}|$. So $D(\omega)$ is the l^1 diameter and $A(\omega)$ is the number of straight internal angles of ω.

Here is the plan of the proof: We will partition the set of all self-avoiding walks of length n into two subsets:

$A = \{\omega$ such that $\omega(0), \omega(N) \notin \{x \in B(\omega) : x_i = m_i\}$ for some $i\}$

$B = \{\omega$ such that the endpoints $\omega(0)$ and $\omega(N)$ are in opposite corners of $B(\omega)\}$.

Note that if ω is not in A then it must be that the endpoints together touch each face of $B(\omega)$ (which is subset B).

If $\omega(0)$ is in subset A, we will show that there exists a pivot point ω_t, and an axis reflection whose result is a SAW ω' with $D(\omega') > D(\omega)$ and $A(\omega') = A(\omega)$. If ω is in subset B and is not a straight rod, we will show that there exists a pivot point ω_s and a 90° rotation (or a diagonal reflection) whose result is a SAW ω' with $A(\omega') = A(\omega) + 1$ and $D(\omega') \geq D(\omega)$. From this, we conclude that for every N step SAW ω that is not a rod, there exists a SAW ω' that may be obtained from ω by a single pivot, and satisfies $A(\omega') + D(\omega') > A(\omega) + D(\omega)$. Since $0 < A < N - 1$ (since there can be at most $N - 1$ straight angles in an N-step self avoiding walk) and $0 < D < N$ for every N-step SAW, and $A + D = 2N - 1$ if and only if the walk is a rod, it follows that any N-step SAW can be transformed into a rod by a sequence of at most $2N - 1$ pivots.

Proof of Theorem 3.1. Case 1: ω is in subset A.

Suppose that there exist $i \in \{1, 2\}$ and $j \in \{1, 2, ..., d\}$ such that neither ω_0 nor ω_N lies in the face $\{x \in B : x_j = m_j^i\}$. Let $t = \min\{k : X_j(\omega_k) = m_j^i\}$. Now reflect $\omega_{t+1}, ..., \omega_N$ through the hyperplane $x_j = m_j^i$, yielding the walk $\omega' = (\omega'_0, ..., \omega'_N)$ defined by:

$$\text{for } k \leq t, w'_k = w_k$$

$$\text{for } k > t, X_l(\omega'_k) = X_l(\omega_k) \text{ for } l \neq j$$

$$X_j(\omega'_k) = 2m_j^i - X_j(\omega_k) \text{ for}$$

We now show that ω' is a self-avoiding walk. We are required to show that for $k > t, \omega'_k$ is not in the set $\{\omega_0, ..., \omega_t\}$. We break it down into two cases:

(i) If $X_j(\omega_k) = m_j^i$, then $\omega'_k = \omega_k$.

(ii) If $X_j(\omega_k) \neq m_j^i$, then $\omega'_k \notin B(\omega)$ therefore, ω'_k is not in $\{\omega_0, ..., \omega_t\}$

Note, that $A(\omega') = A(\omega)$ since right angles are preserved by axis reflections. Now, we show that $D(\omega') > D(\omega)$. Observe that $M_l(\omega') = M_l(\omega)$ for $l \neq j$.

Define $Q_{r,s}(\omega)$ be the extension in the jth coordinate direction of the subwalk $\omega_r, \omega_{r+1}, ..., \omega_s$, i.e., $Q_{r,s}(\omega) = \max\{X_j(\omega_k) : r \leq k \leq s\} - \min\{X_j(\omega_k) : r \leq k \leq s\}$.

Then, $M_j(\omega) = \max(Q_{0,t}(\omega), Q_{t,N}(\omega))$ while, $M_j(\omega') = Q_{0,t}(\omega) + Q_{t,N}(\omega)$

By definition, $Q_{0,t}(\omega)$ and $Q_{t,N}(\omega)$ are strictly positive so $M_j(\omega') > M_j(\omega)$. Hence, $D(\omega') > D(\omega)$.

Case 2: ω is in subset B and is not a rod. Then $A(\omega) < N - 1$, i.e., ω contains at least one right angle, so we choose our pivot point ω_s to be the last right angle of ω, i.e., $s = \max\{k : 0 < k < N, w_k \neq \frac{1}{2}(\omega_{k-1} + \omega_{k+1})\}$. Thus $(\omega_s, \omega_{s+1}, ..., \omega_N)$ lie on a straight line perpendicular to the line segment joining ω_{s-1} with ω_s. Let j' and j" be the (unique) coordinates satisfying $X_{j'}(\omega_s) \neq X_{j'}(\omega_N)$ and $X_{j"}(\omega_{s-1}) \neq X_{j"}(\omega_s)$. Now perform a 90° rotation (or diagonal reflection) at j' to get a new SAW ω' with $\omega'_k = \omega_k$ for $k \leq s$, and $(\omega_{s-1}, \omega_s, ..., \omega_N)$ all on one straight line. Since $\omega'_{s+1}, ..., \omega'_N \in B(\omega)$, ω' is a SAW.

Note that choosing the above pivot increases the number of straight-line angles by 1, i.e., $A(\omega') = A(\omega) + 1$. From above, we also get that the j''^{th} coordinate of the new walk increases by $N - s$. Thus, $M_{j''}(\omega') = M_{j''}(\omega) + (N - s)$. Also, $M_{j'}(\omega') \geq M_{j'}(\omega) - (N - s)$ since the j'^{th} coordinate decreases at most by $N - s$ from the old walk. $M_j(\omega') = M_j(\omega)$ for all other $j \in \{1, 2, ..., d\}$. Thus, $D(\omega') \geq D(\omega)$.

Next we prove that the pivot algorithm is aperiodic.

Take an n step self-avoiding walk starting at the origin at the i^{th} implementation of the algorithm. Let $\Lambda = \{n : p^n_{(i,i)} > 0\}$. By rotating the walk 4 times by 90° degrees we would get back the walk we started with. Thus $4 \in \Lambda$. Again, we can get the walk in 3 steps by rotating it first by 180° and then by doing 290° rotations, thus, $3 \in \Lambda$. Since the period of a markov chain is the greatest common divisor of Λ, so the period is 1. Since we took an arbitrary state, the pivot algorithm is aperiodic.

Therefore, the pivot algorithm is ergodic.

□

5.3 Proof of Theorem 3.2

Here we show that even if axis reflections are not there in 2 dimensions, the pivot algorithm is ergodic.

Proof of Theorem 3.2. It is enough to show that any ω with $A(\omega) < N - 1$ can be transformed into a self-avoiding walk ω' with $A(\omega') = A(\omega)+1$ by some finite sequence of allowed pivots. Let ω be an N-step SAW. Then WLOG, assume that ω_N and ω_{N-1} differ on the y coordinate,i.e. $\omega_N = \omega_{N-1} \pm (0, 1)$. If $m^1_1(\omega) = m^2_1(\omega)$, i.e. the maximum of the x coordinate is equal to the minimum of the x coordinate, then, ω is a straight rod. So, assume that $m^1_1 < m^2_1$. Choose $i \in \{1, 2\}$ so that $X_1(\omega_0) \neq m^i_1$.

Case 1. If $X_1(\omega_N) = m^i_1$, then let ω_s be the last right angle in ω, i.e., $s = \max\{k : 0 < k < N, \omega_k \neq \frac{1}{2}(\omega_{k-1} + \omega_{k+1})\}$. Then a 90° rotation (or a diagonal reflection) at ω_s gives a new walk ω' in which $\omega'_s, ..., \omega'_N$ lie on a straight line $x_2 =$ constant, and $A(\omega') = A(\omega) + 1$.

Case 2. If $X_1(\omega_N) \neq m^i_1$, let $z = \min\{x_2 : (m^i_1, x_2) \in \{\omega_0, ..., \omega_N\}\}$ and let t be the unique index such that $\omega_t = (m^i_1, z)$. We can rotate the walk by 180° at ω_t, to get a new SAW ω'' with $X_1(\omega_{N-1}) = X_1(\omega_N)$. Again, $A(\omega'') = A(\omega)$ since rotation by 180° doesn't change the number of straight line angles. Again, $M_1(\omega'') > M_1(\omega)$. We now repeat this procedure; after at most N 180° rotations we will be in case 1, and hence able to increase A by 1. □

6 Acknowledgement

I extend my sincere gratitude to my supervisor, Prof. Siva Athreya, for his invaluable assistance and support during my participation in this summer program. I am immensely thankful to the ICTS - S.N.Bhatt Memorial Excellence Fellowship Program - 2023 for providing me with the opportunity to interact with esteemed professors and fellow students at ICTS this summer. Lastly, I would like to thank my friends and family for their constant support throughout my academic pursuits.

References

[1] Paul J Flory. *Principles of polymer chemistry*. Cornell university press, 1953.

[2] Eugene Guth. Theory of filler reinforcement. *Rubber Chemistry and Technology*, 18(3):596–604, 1945.

[3] John M Hammersley and K William Morton. Poor man's monte carlo. *Journal of the Royal Statistical Society: Series B (Methodological)*, 16(1):23–38, 1954.

[4] Brian Hayes. Computing science: How to avoid yourself. *American Scientist*, 86(4):314–319, 1998.

[5] Wyatt Hooper and Alexander R Klotz. Trapping in self-avoiding walks with nearest-neighbor attraction. *Physical Review E*, 102(3):032132, 2020.

[6] Jesper Lykke Jacobsen, Christian R Scullard, and Anthony J Guttmann. On the growth constant for square-lattice self-avoiding walks. *Journal of Physics A: Mathematical and Theoretical*, 49(49):494004, 2016.

[7] Werner Kuhn. Beziehungen zwischen molekülgröße, statistischer molekülgestalt und elastischen eigenschaften hochpolymerer stoffe. *Kolloid-Zeitschrift*, 76(3):258–271, 1936.

[8] Neal Madras and Gordon Slade. *The self-avoiding walk*. Springer Science & Business Media, 2013.

[9] Neal Madras and Alan D Sokal. The pivot algorithm: a highly efficient monte carlo method for the self-avoiding walk. *Journal of Statistical Physics*, 50:109–186, 1988.

[10] Berenike Maier and Joachim O Rädler. Conformation and self-diffusion of single dna molecules confined to two dimensions. *Physical review letters*, 82(9):1911, 1999.

[11] WJC Orr. Statistical treatment of polymer solutions at infinite dilution. *Transactions of the Faraday Society*, 43:12–27, 1947.

[12] Andrea Pelissetto and Jean-Pierre Hansen. Corrections to scaling and crossover from good-to θ-solvent regimes of interacting polymers. *The Journal of chemical physics*, 122(13):134904, 2005.

[13] Gordon Slade. Self-avoiding walks. *The Mathematical Intelligencer*, 16(1):29–35, 1994.

[14] Gordon Slade. The self-avoiding walk: A brief brief survey. *Surveys in Stochastic Processes*, 4:181, 2011.