PATTERN THEOREM FOR THE HEXAGONAL LATTICE

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Contents

Summary

A linear polymer can be thought of as a flexible long chain of beads that follows a lattice where each bead represents a monomer unit. It can be modelled as a self-avoiding random walk on a lattice. When the linear polymer is in a chemical solution and is following a 2-dimensional hexagonal lattice, it becomes self-entangled. It can be shown that in all sufficiently long polymers a pattern is present. Kesten's Pattern Theorem, which was originally proved for self-avoiding walks on cubic lattices, is extended to the self-avoiding walks on hexagonal lattices. Properties of the hexagonal lattice, self-avoiding walks on the hexagonal lattice and the connective constant for the hexagonal lattice are then provided. Further, computation of the probability of a self-avoiding walk on the hexagonal lattice encircling the points $(\frac{1}{2}, \frac{1}{2})$ and $(\frac{1}{2}, -\frac{1}{2})$ is discussed.

List of Tables

List of Figures

List of Notations

c_N	Number of N-step self-avoiding walks starting at origin
γ	Kesten's pattern
μ	Connective constant
$\mathbb{H}$	Hexagonal lattice
H	Hexagonal ball of no specified size
H_n	Hexagonal ball of size n
l_i	i-th layer of the hexagonal ball H_n
r_n	Radius of Euclidean circle centred at H_0, circumscribing the hexagonal ball H_n
ω	Self-avoiding walk
ω_N	N-step self-avoiding walk
$\omega(i)$	i-th step of the self-avoiding walk ω
$H_n(j)$	n-layered hexagonal ball centered at $\omega(j)$, enclosed by circle of radius r_n
$\overline{\omega}(i)$	i-th trajectory of the self-avoiding walk ω

S_N	Set of N-step self-avoiding walk with initial point at origin
E^*	Event that $H_n(j)$ is completely covered by ω
E_k	Event that at least $k \geq 1$ lattice points of $H_{n+2}(j)$ are covered by ω
$\tilde{E}_k$	Event that occurs at $\omega(j)$ if E^* or E_k or both occur there
E	Any of the events E^*, E_k or $\tilde{E}_k$
$E(m)$	Event that E occurs at m-th step of ω_{2m}
$c_N[k, E]$	# of self-avoiding walks in S_N where E occurs at no more than k different steps
$c_N[k, E(m)]$	# of self-avoiding walks in S_N where $E(m)$ occurs at no more than k different steps
$c_N[k, (\gamma, H_n)]$	# of self-avoiding walks in S_N where (γ, H_n) occurs at no more than k different steps

Chapter 1

Introduction

A polymer is a large molecule composed of many small, simple chemical units, or monomers, joined together by chemical bonds. The structural properties of a polymer are related to the physical arrangement of monomers along the chain. Long chain linear polymers composed of a large number of units display properties that are completely different from short chain polymers composed of fewer units. For example, two samples of natural rubber may exhibit different durability even though they are made up by the same monomers. The structure has a strong influence on the physical properties of a polymer and these can be understood through statistical mechanics. A linear polymer chain has a high degree of flexibility. We can think of it as a very long chain of beads where we can assume that the chain follows a lattice, that is, each bead represents a monomer unit and occupies a lattice site adjacent to the monomer units to which it is attached. When a polymer molecule is dissolved in a solvent, the

entire molecule forms a coil structure with a large number possible folding shapes, because of the high flexibility of the chemical bonds that connect the atoms.

1.1 Modelling a Polymer

Let us assume that there is no correlation between the directions that different chemical bonds take and all the directions have the same probability. Then the configuration of a polymer may be modelled as a random walk on a lattice and hence we can find out properties of the polymer molecule by using the properties of a random walk on the lattice structure. This would describe an ideal chain polymer model. The configuration of an ideal chain, with no interactions between monomers, is the essential starting point of most models in polymer physics. In an ideal model, fixed length polymer segments are linearly connected and all bonds and angles between the bonds are equiprobable. In the ideal chain polymer, there are no interactions between monomers that are far apart along the chain even if they approach each other in space. This situation is never completely realized for real chains. The ideal model takes place only in short range interactions between segments which are located close to each other along the chain. This model allows a chain to loop back onto itself. It means that the segments which are widely separated along the chain will occupy the same region in space. This is a physical impossibility since each segment possesses its own finite volume and two segments cannot occupy the same region in space. This type of condition is called the *excluded volume effect*. Real chains interact with both

their solvent and themselves. The relative strength of these interactions determines whether the monomers effectively attract or repel one another. When we model a polymer as a connected path on a lattice, the excluded volume effect will correspond to the condition that the path cannot pass through any sites that have been traversed previously. This is called a *self-avoiding walk* and the polymer thus represented is called an excluded volume chain. To get the idea about polymers, one can see [5] and [18]. Self-avoiding walks on regular lattices have been studied for many years as a model of linear polymer molecules in dilute solution. Self-avoiding walks have a high degree of conformational freedom, and it ensures non-occupation of the same volume space by more than one monomer unit in the polymer. A walk is a directed sequence of edges, such that adjacent pairs of edges in the sequence are incident on a common vertex. A walk is self-avoiding if no vertex is visited more than once. Two walks are considered distinct if they cannot be super-imposed by translation. For more properties of a self-avoiding walk, one can see [14] and [15].

There are rigorous results proving that almost all sufficiently long polymers are knotted. A knot is created by beginning with a one-dimensional line segment, wrapping it around itself arbitrarily, and then fusing its two free ends together to form a closed loop. It is of interest to know how many different configurations an n-monomer chain can adopt and how far apart the end points of the molecule typically are. These problems can be viewed as problems of self-avoiding random walk in an appropriate lattice.

The idea to show that all sufficiently long polymers are knotted falls into three parts. The first is a pattern theorem by Kesten in [13]. A pattern is a finite self-avoiding walk that occurs as part of a longer self-avoiding walk. Given a particular pattern γ, if there exists a self-avoiding walk on which the pattern γ appears at least three times, then we call γ a K-pattern. The point of appearing three times is that one of the occurrences must be "between" the other two, and hence there must be a way in to the beginning of the patern and a way from the end.

Let c_N denote the number of N-step self-avoiding walks, which begin at the origin. This measures the number of possible configurations of a polymer of $(N+1)$ monomers. It can be shown that $\lim_{N\to\infty} c_N^{\frac{1}{N}}$ exists. Let us take the limit as, $\lim_{N\to\infty} c_N^{\frac{1}{N}} = \mu$, where we define μ as the connective constant for that particular molecular lattice. When the self-avoiding walk is on a cubic lattice, there are rigorous results for the relations between c_N and μ in [13] and [15]. Kesten's Pattern Theorem can be used to prove some useful results for the square lattice structures. For 2-dimensional honeycomb lattice there is strong evidence from physical arguments in [16] that $\mu = \sqrt{2+\sqrt{2}}$. This value has been confirmed numerically, but not yet by a rigorous proof. In this thesis, we have tried to see whether the theorems and results which are applicable for a square lattice can be extended to a honeycomb lattice.

1.2 Organization of the Thesis

In Chapter 2 of this thesis we define a hexagonal lattice, and show how to generate the hexagonal lattice. The definition of a self-avoiding walk and its trajectory remains similar to that for a square lattice. For the hexagonal lattice, we have given the values of c_N for $N = 1, \cdots, 14$, an upper and lower bound for c_N and seen that the subadditive property of c_N also holds. We have also given the definitions of a pattern, proper internal pattern and a self-avoiding N-loop in this chapter.

In Chapter 3, we have discussed about a few results of [22] which are the motivation behind this thesis. Kesten's pattern theorem which is the very first step to see if a long chain polymer is knotted, is proved for square molecular lattice structure by Kesten in [13]. The basic idea of Kesten's pattern theorem is, if a given pattern can possibly occur several times on a self-avoiding walk, then it must occur at least aN times on on all N-step self-avoiding walks, except for an exponentially small fraction of the walk. We have extended the pattern theorem and a few lemmas and conclusions related to this theorem to the hexgonal lattice.

Dubins *et al.* in [6] have shown that the probability that a N-step self-avoiding random loop in a square lattice structure, contains the point $(\frac{1}{2}, \frac{1}{2})$ is $\frac{1}{2} - \frac{1}{N}$. In Chapter 4, we have discussed similar results for a N-step self-avoiding random loop in a hexagonal lattice structure and have found out that the probability that the point $(\frac{1}{2}, \frac{1}{2})$ is inside is $\frac{1}{2} - \frac{1}{N}$. We have also seen that the probability that a N-step self-avoiding random loop on a hexagonal lattice will contain the points $(\frac{1}{2}, \frac{1}{2})$ and

$(\frac{1}{2}, -\frac{1}{2})$ is $\frac{1}{6} - \frac{1}{N}$.

In appendix C, we have given a MAPLE code which we have used to calculate the results in Table 2.1.

Chapter 2

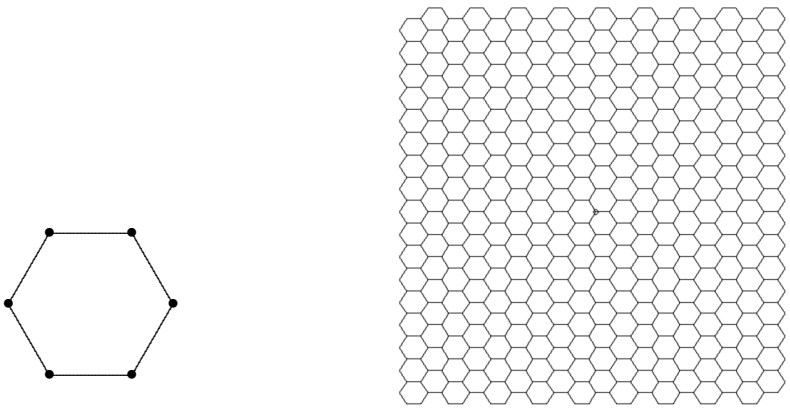
Hexagonal Lattice

There are various results for the cubic lattice regarding the structure of the lattice, the number of N-step self-avoiding walks c_N and connective constant μ. We now extend some of those results to the hexagonal lattice structures. For that, we need to introduce a few definitions and notations for the hexagonal lattice.

2.1 Hexagonal Lattice and Some Properties

A hexagon is a polygon with six edges and six vertices. The internal angles of a regular hexagon (one whose all sides and all angles are equal) are all 120^o. It has 6 lines of symmetry. Like squares and equilateral triangles, regular hexagons fit together without any gaps to tile the plane (three hexagons meeting at every vertex). The resulting lattice is called the **hexagonal lattice**. Denote the hexagonal lattice by $\mathbb{H}$ and suppose that the length of the edge joining adjacent vertices are one unit.

Define a **unit hexagon** as a regular hexagon with unit side length. We now introduce



(a) Regular Hexagon (b) Hexagonal Lattice $\mathbb{H}$

Figure 2.1: Regular Hexagon and Hexagonal lattice

the idea of layers as follows, which is done recursively.

Definition 2.1.1 *Consider a lattice point H_0 in $\mathbb{H}$. Define it as the **0-th layer** or l_0 for a hexagonal ball as in Figure 2.2. Suppose that the hexagonal ball, H_n has been defined. Then define the $(n+1)$-th layer l_{n+1} as the set of all lattice points belonging to at least one unit hexagon in $\mathbb{H}$ which has at least one vertex common with H_n. Then define*

$$H_{n+1} = H_n \cup l_{n+1} \tag{2.1}$$

Note:

1. H_n is a hexagonal ball of size n (i.e. it has $n+1$ layers), centered at H_0, i.e.

$$H_n = \bigcup_{i=0}^{n} l_i.$$

2. A lattice point x belongs to a **layer** n around H_0 if it belongs to a unit hexagon touching the layer $(n-1)$ around point H_0, but does not belong to that layer $(n-1)$ itself. For example, the hexagonal ball with only one layer, H_1 is shown

Figure 2.2: 0-th layer of a hexagonal ball

in Figure 2.3.

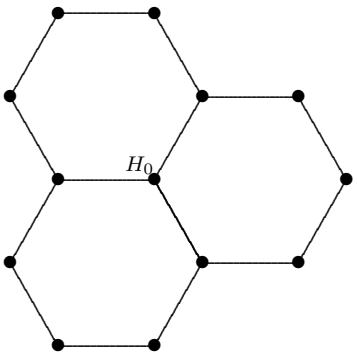


Figure 2.3: H_1

3. We denote by H a hexagonal ball whose size is not specified.

Definition 2.1.2 *A Euclidean circle centered at H_0 with radius $r_n = \sqrt{1+3n^2}$ units will enclose all points of the n-layered hexagonal ball H_n. The circle is called the* ***circumscribing circle*** *of H_n.*

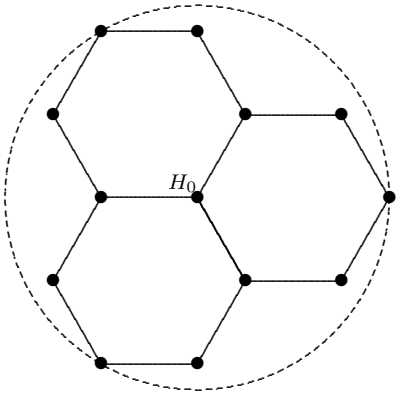


Figure 2.4: Circumscribing circle of H_1 with radius $r_1 = 2$

Note:

1. In Figure 2.4 the dotted circle is circumscribing H_1 where the radius of the circle is $r_1 = 2$. Suppose, H_n is an n-layered hexagonal ball centered at $H_0 = y$(say). We define the following,

$$\begin{aligned} H_n &= \{x \in \mathbb{H} : |x - y| \leq r_n\} \\ H_{n+1} &= \{x \in \mathbb{H} : |x - y| \leq r_{n+1}\}. \end{aligned}$$

The following equation (2.2) is another way to define the n-layer hexagonal ball H_n and $(n+1)$-th layer of the hexagonal ball, l_{n+1}, using the circumscribing

circle.

$$l_{n+1} = H_{n+1} \setminus H_n. \tag{2.2}$$

We have shown that the two definitions of layers are the same in appendix A.

(a) (b)

Figure 2.5: Two types of possible origins in a hexagonal lattice

2. Note that, as shown in Figure 2.5, we can have two types of configuration for a center of a hexagonal ball. These two orientations may seem to be different as they cannot be superimposed on each other by translation. If we use rotation and reflection, then we can superimpose them.

Proposition 2.1.1 *The hexagonal lattice can be generated by the following set,*

$$\begin{aligned} \mathbb{H} &= \{\lambda_1\vec{e_1} + \lambda_2\vec{e_2} \in R^2 : \lambda_1 + \lambda_2 \not\equiv 2(mod\,3), \lambda_1, \lambda_2 \in Z\} \qquad (2.3) \\ where\ \vec{e_1} &= \vec{i} \\ and\ \vec{e_2} &= -\frac{1}{2}\vec{i} + \frac{\sqrt{3}}{2}\vec{j} \end{aligned}$$

Proof: We will give an outline to generate the hexagonal lattice. Let us take $O(0,0)$ as the origin and let $\vec{e_1}$ and $\vec{e_2}$ be two unit vectors along the two edges of the hexagon

where the angle between $\vec{e_1}$ and $\vec{e_2}$ is 120^o. In Figure 2.6, we have taken $\vec{e_1}$ along $\vec{OA}$ and $\vec{e_2}$ along $\vec{OB}$. Now we are trying to span the hexagonal lattice using $\vec{e_1}$ and $\vec{e_2}$. We can see that the centers of the hexagons (in the Figure 2.6, the centers are,

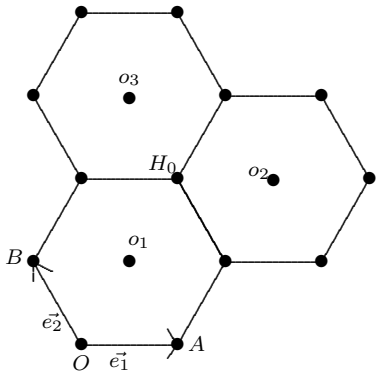


Figure 2.6: Spanning a hexagonal ball

o_1, o_2 and o_3), which are not part of the lattice can be generated by the following expression.

$$m(\vec{e_1} + 2\vec{e_2}) + n(2\vec{e_1} + \vec{e_2}) - \vec{e_2} = (m + 2n)\vec{e_1} + (2m + n - 1)\vec{e_2}, \tag{2.4}$$

where m and n are integers.

The derivation of (2.4) is provided in appendix B. Now, if $\vec{a} = (\lambda_1\vec{e_1} + \lambda_2\vec{e_2})$ is the position vector of a center of a hexagon, then, we have,

$$\begin{aligned} \lambda_1 &= m + 2n, \\ \lambda_2 &= 2m + n - 1. \end{aligned}$$

So, $3n = 2\lambda_1 - \lambda_2 - 1$, and hence to generate the centers of a hexagon the required condition is that $3|(2\lambda_1 - \lambda_2 - 1)$ as m, n are integers. Thus the condition on λ_1 and λ_2 to generate hexagonal lattice is that $2\lambda_1 - \lambda_2 \not\equiv 1(mod\,3)$, which can be simplified to

$$\lambda_1 + \lambda_2 \not\equiv 2(mod\,3).$$

Hence we can span the hexagonal lattice as described by proposition 2.1.1.

□

2.2 Self-avoiding Walks on a Hexagonal Lattice

To define a N-step self-avoiding walk, we first define a *step* in a hexagonal lattice.

Definition 2.2.1 *A **step** is defined as an element of* $\{\pm\vec{e_1}, \pm\vec{e_2}, \pm(\vec{e_1} + \vec{e_2})\}$. *A **walk** is a finite sequence of steps. The **length** of a walk is the number of steps in the lattice. A walk of length N is an **N-walk**. So, if we have a walk,* $\omega = \{\omega(0), \cdots, \omega(N-1)\}$ *in* $\mathbb{H}$, *then,* $(-1)^i\omega(i) \in \{\vec{e_1}, \vec{e_2}, -(\vec{e_1} + \vec{e_2})\}$ *and as ω has N elements, hence it is an N-walk.*

We need at least one step for a walk.

Definition 2.2.2 *Let,* $\omega = \{\omega(0), \cdots, \omega(N-1)\}$ *be an N-walk. The **trajectory** of the walk is defined as the sequence* $\overline{\omega} = \{\overline{\omega}(0), \cdots, \overline{\omega}(N-1)\}$ *defined by* $\overline{\omega}(0) = \vec{0}$ *and* $\overline{\omega}(j) = \omega(0) + \cdots + \omega(j)$, *for* $1 \leq j \leq N-1$.

Definition 2.2.3 *Let, $\omega = \{\omega(0), \cdots, \omega(N-1)\}$ be an N-walk. Then, ω is a* ***self-avoiding walk*** *if,*

$$\begin{aligned} \sum_{k=0}^{i} \omega(k) &\neq \sum_{k=0}^{j} \omega(k), \forall i \neq j \\ \iff \overline{\omega}(i) &\neq \overline{\omega}(j), \forall i \neq j. \end{aligned}$$

In other words, we can say that a self-avoiding walk is a walk from one lattice point to another along the lattice which never intersects itself. So, we denote a self-avoiding walk by ω, a step of the self-avoiding walk by $\omega(i)$ and the i-th trajectory of the self-avoiding walk by $\overline{\omega}(i)$. Let $\omega = (\omega(0), \cdots, \omega(N-1))$ be a N-step self-avoiding walk on the hexagonal lattice $\mathbb{H}$ and suppose that H_n is an n-layered hexagonal ball in $\mathbb{H}$ centered at $\omega(j)$, where $\omega(j)$ denotes the j-th step of ω. For $j = 0, 1, \cdots, N$, we denote

$$H_n(j) = \{x \in \mathbb{H} : |x - \omega(j)| \leq r_n\}.$$

2.2.1 On Number of N-step Self-avoiding Walks

Let S_N denote the set of N-step self avoiding walks ω such that $\overline{\omega}(0) = \vec{0}$. Let us denote by $|S_N| = c_N$, i.e. c_N is the number of N-step self-avoiding walks which begin at the origin.

Now suppose that ω_1 and ω_2 are two M-step and N-step self-avoiding walks respectively. Then, the *concatenation* of ω_1 and ω_2, which we denote by ω, can be

defined in terms of its trajectory as follows,

$$\begin{aligned}\overline{\omega}(k) &= \overline{\omega_1}(k),\ k = 0, \cdots, M-1;\\ \overline{\omega}(k) &= \overline{\omega_2}(k-M) + \overline{\omega_1}(N) - \overline{\omega_2}(0),\ k = M, \cdots, M+N-1.\end{aligned}$$

Proposition 2.2.1 *Let c_M, c_N and c_{N+M} be the cardinalities of the set of self-avoiding walks of length M, N and $(N+M)$ respectively. Then*

$$c_{N+M} \leq c_N c_M. \tag{2.5}$$

Proof: Since c_M and c_N are the cardinalities of the set of self-avoiding walks of length M and N respectively, the product $c_N c_M$ is equal to the cardinality of the set of $(N+M)$-step walks which are self-avoiding in the initial N-step and the final M-steps, but which may not be completely self-avoiding. Hence, by concatenation of M-step walks to N-step walks, we can say that,

$$\begin{aligned}S_{N+M} &\leq S_N \cup S_M\\ \Rightarrow |S_{N+M}| &\leq |S_N||S_M|\\ \Leftrightarrow c_{N+M} &\leq c_N c_M.\end{aligned} \tag{2.6}$$

Thus the sequence $\{c_q\}$ is *submultiplicative*. □

So, by (2.6) and taking logarithm, we have,

Corollary 2.2.1

$$log\ c_{N+M} \leq log\ c_N + log\ c_M, \tag{2.7}$$

i.e. the sequence $\{log\ c_q\}$ *is subadditive.*

We now introduce a property for a sequence of subadditive real numbers, which is proved in [14] and [15]. The result is shown in lemma 2.2.1.

Lemma 2.2.1 *Let* $\{p_N\}_{N\geq 0}$ *be a sequence of real numbers which is subadditive, i.e.,* $p_{N+M} \leq p_N + p_M$. *Then the* $\lim_{N\to\infty} \frac{p_N}{N}$ *exists in* $[-\infty, \infty)$. *Also,*

$$\lim_{N\to\infty} \frac{p_N}{N} = \inf_{N\geq 1} \frac{p_N}{N}. \tag{2.8}$$

Proof: It is clear that

$$\liminf_{N\to\infty} \frac{p_N}{N} \geq \inf_{N>0} \frac{p_N}{N}. \tag{2.9}$$

To prove (2.8), it is sufficient to show that,

$$\limsup_{N\to\infty} \frac{p_N}{N} \leq \frac{p_k}{k}, \forall k. \tag{2.10}$$

Fix k. Let,

$$P_k = \max_{1\leq r\leq k} p_r.$$

Let N be a positive integer, and j be the largest integer strictly less than $\frac{N}{k}$. Then,

$N = jk + r$, for $1 \leq r \leq k$, where r is an integer. By subadditivity,

$$p_N \leq jp_k + p_r \leq \frac{N}{k} p_k + P_k. \tag{2.11}$$

Dividing (2.11) by N, we have,

$$\frac{p_N}{N} \leq \frac{j}{N} p_k + \frac{p_r}{N} \leq \frac{1}{k} p_k + \frac{P_k}{N}. \tag{2.12}$$

Hence (2.10) follows by taking limsup as $N \to \infty$. □

Hence by lemma 2.2.1, we can see that $\lim_{N\to\infty} c_N^{\frac{1}{N}}$ exists. Now,

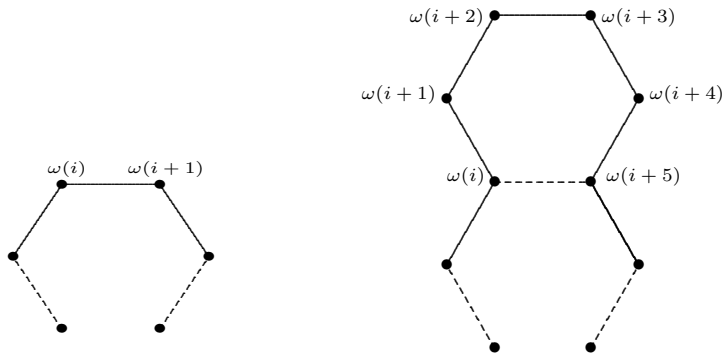
Proposition 2.2.2 *For a self-avoiding N step walk ω, in the lattice $\mathbb{H}$,*

$$c_N \leq c_{N+4}. \tag{2.13}$$

Idea of the proof: The idea to show (2.13) is to increase the length of an N-step self-avoiding walk by 4. Suppose ω is a N-step self-avoiding walk on n-layered hexagonal ball H_n. Let,

$$\begin{aligned} H_{(n)} &= \max\{H_i : \text{ at least one } \omega(i) \in H_i, \text{ for } i = 1, \cdots, n\} \\ l_{(n)} &= \text{ outer most layer of } H_{(n)} \\ K &= \max\left\{n : \overline{\omega}(i) \in l_{(n)} \text{ , for some } i\right\}. \end{aligned}$$

Then ω can be extended to $\tilde{\omega} \in S_{N+4}$ within H_{K+1} by adding 4 steps to ω. Now we



(a) N-step self-avoiding walk

(b) $(N+4)$-step self-avoiding walk

Figure 2.7: Augmenting a self-avoiding random walk by 4 steps

join two lattice points from H_{K+1} to ω in the following way,

$$\begin{aligned}
\overline{\omega}(i+1) &= \overline{\omega}(i) + \vec{e}_2 \\
\overline{\omega}(i+2) &= \overline{\omega}(i+1) + (\vec{e}_1 + \vec{e}_2) \\
\overline{\omega}(i+3) &= \overline{\omega}(i+2) + \vec{e}_1 \\
\overline{\omega}(i+4) &= \overline{\omega}(i+3) - \vec{e}_2 \\
\overline{\omega}(i+5) &= \overline{\omega}(i+4) - (\vec{e}_1 + \vec{e}_2).
\end{aligned}$$

So, we get a $(N+4)$-step self-avoiding walk on the lattice. Hence, we have (2.13). □

An interesting question would be to find out about the values of c_N for various values of N for a hexagonal lattice. We define $c_0 = 1$.

In Table 2.1 we can see the values of c_N for different values of N. This has been

N	c_N
1	3
2	6
3	12
4	24
5	48
6	90
7	174
8	336
9	648
10	1218
11	2328
12	4416
13	8838
14	15780

Table 2.1: Number of self-avoiding walks for different step lengths

found out by using MAPLE. The codes are given in appendix B. Since $\lim_{N\to\infty} c_N^{\frac{1}{N}} = \log \kappa$ (say) exists, we can say that

$$c_N \sim \ ce^{\kappa N}$$

for some $c > 0$ for large N.

We can find out upper and lower bounds for c_N. A simple way to estimate a crude upper and lower bound for c_N is given by the following proposition.

Proposition 2.2.3 *For an N-step self-avoiding walk on a hexagonal lattice,*

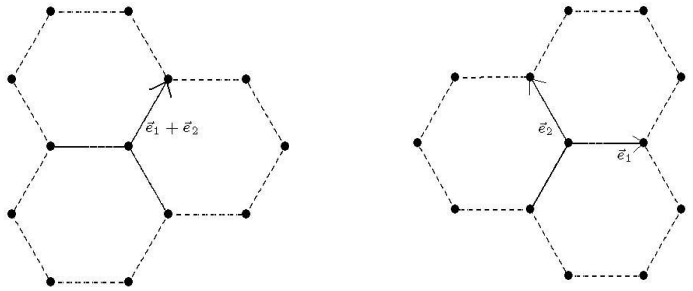
$$2^{\frac{N}{2}} \leq c_N \leq 3 \times 2^{N-1}. \tag{2.14}$$

Proof: The upper bound of c_N is given by the number of walks ω which never visit the same site at steps $\omega(i)$ and $\omega(i+2)$. At the first step of ω, we can move along the direction of either of the three basis vectors, $\vec{e_1}, \vec{e_2},$ or $-(\vec{e_1} + \vec{e_2})$. So, we have 3 choices for the first step of ω. At the second step of ω, as the walk is self-avoiding, we have 2 choices. So we are having 2 choices for each of the remaining $N-1$ steps. Thus, as upper bound of c_N we have,

$$c_N \leq 3 \times 2^{N-1}. \tag{2.15}$$

We can also have a lower bound for c_N. To find a lower bound, we apply a few restrictions on the self-avoiding walk on the hexagonal lattice $\mathbb{H}$. Here we will always move forward or upward at each lattice point. In a lattice point like Figure 2.8 (a), we allow the walk to move only upwards, i.e. along the direction of $(\vec{e_1} + \vec{e_2})$. When the lattice point configuration is like Figure 2.8(b), then we have two choices, which are moving forward or moving upward, i.e. along the direction $\vec{e_1}$ or along direction $\vec{e_2}$. So

our *Type 1* choice would be moving along $(\vec{e}_1 + \vec{e}_2)$ direction and *Type 2* choice would be moving along either $\vec{e}_1$ direction or along $\vec{e}_2$ direction. From the hexagonal lattice



(a) (b)

Figure 2.8: Lower bound for c_N

structure we can see that the *Type* 1 choice and the *Type* 2 choice occur alternatively at each lattice points. Hence, the *Type* 2 choice occurs $\frac{N}{2}$ number of times. So,

$$2^{\frac{N}{2}} \leq c_N. \tag{2.16}$$

Hence, we get (2.14), the upper and lower bounds for c_N from (2.15) and (2.16) □

As $\lim_{N\to\infty} c_N^{\frac{1}{N}}$ exists by lemma 2.2.1, we can have the following corollary,

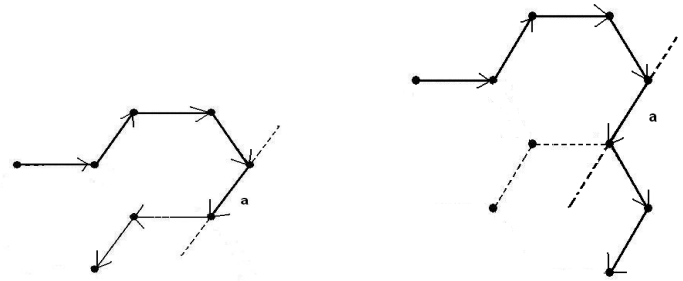
Corollary 2.2.2

$$2^{\frac{1}{2}} \leq \lim_{N\to\infty} c_N^{\frac{1}{N}} \leq 2. \tag{2.17}$$

2.2.2 Further Discussion on the Bounds on c_N

We can improve the upper bound in (2.14) further. Suppose we are unfolding our self-avoiding walk to make it a restricted walk. The unfolding is done with the help

of reflection along a side joining two adjacent lattice points on the lattice $\mathbb{H}$. The rule is that, we do not reflect as long as we are going forward, upward or downward. But suppose we have a segment of the path which goes backward. We will then reflect the rest of the self-avoiding walk along the segment which is just before the segment which goes backwards. In Figure 2.9(a), we are reflecting along a to get Figure 2.9(b). Now



(a) Before reflection (b) After reflection along a

Figure 2.9: Reflecting and unfolding of a self-avoiding walk

we record the positions of the segments along which an N-step self-avoiding random walk needs to be reflected to get a restricted walk. Equivalently, we are trying to find the number of possible ways of partitioning the number N. For example, if we need to reflect a 20-step self-avoiding walk at the 5-th, 7-th and 10-th segment, then, the corresponding partition would be $\{5, 2, 3, 10\}$. Hardy and Ramanujan in [12] showed that $R(N)$, the number of partitioning of the number N is,

$$R(N) \approx \frac{\exp(\pi\sqrt{\frac{2N}{3}})}{4N\sqrt{3}}. \tag{2.18}$$

As we are partitioning the set S_N, as described above, we get,

$$\begin{aligned} S_N &= \sqcup_{R(N)} S_{R(N)} \\ \text{where, } S_{R(N)} &= \text{set of elements in each partition.} \end{aligned} \tag{2.19}$$

Hence, from (2.19), we have,

$$|S_N| = c_N = \sum_{R(N)} |S_{R(N)}| \leq R(N) \times 2^{\frac{N}{2}} \tag{2.20}$$

as we have seen the restricted walk which goes only forward and upward has $2^{\frac{N}{2}}$ possibilities. So from (2.20), we get,

$$c_N \leq R(N) \times 2^{\frac{N}{2}} < 2^N \tag{2.21}$$

for large N. Hence we get a better upper bound smaller than 2 which means that the bounds on c_N can be further improved by restricting self-avoiding walks on the hexagonal lattice.

2.3 Patterns and Random Loops

In this section we define patterns and self-avoiding loops. Patterns can be described as self-avoiding walks which appear as a sub-walk in a longer self-avoiding

walk.

Definition 2.3.1 *A* ***pattern*** $\gamma = (\gamma(0), \cdots, \gamma(M))$ *is a self-avoiding walk and it is said to occur at the j-th step of the self-avoiding walk* $\omega = (\omega(0), \cdots, \omega(N-1))$ *if* $\omega(j+k) = \gamma(k), \forall k = 0, \cdots, M$.

Definition 2.3.2 *Let us suppose that* H *is a hexagonal ball and* γ *is a pattern such that it is totally contained inside* H*, there is a way into to the hexagonal ball* H *to* γ *and there is a way out from* γ *and from* H*. Then we can say that* γ *is a* ***proper internal pattern****.*

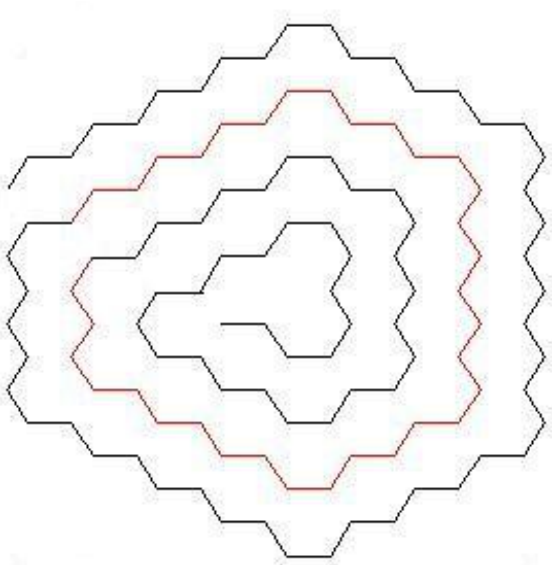


Figure 2.10: A pattern which is not a proper internal pattern

Figure 3.1 in Chapter 3, represents a proper internal pattern on a hexagonal lattice. There can also be patterns which are not proper internal patterns. One example is

given Figure 2.10.

Suppose that H_n is an n-layered hexagonal ball and $\gamma = (\gamma(0), \cdots, \gamma(M))$ is an M-step pattern such that $\gamma(0)$ and $\gamma(M)$ are one of the n-th layer lattice points of H_n, and $\gamma(i) \in H_n, \forall i = 0, \cdots, M$, i.e., γ is a proper internal pattern. Then we define the following,

Definition 2.3.3 *(γ, H_n) denotes a pair which consists of a proper internal pattern γ and the hexagonal ball H_n. (γ, H_n) occurs at the j-th step of the self-avoiding walk ω if $\omega(j+k) = \gamma(k)$ for every $k = 0, \cdots, M$, and $\omega(i)$ is not in H_n for every $i < j$ and every $i > j + M$.*

Let $c_N[k, \gamma]$ denote the number of self-avoiding walks in S_N for which γ occurs at no more than k different steps, for $k \geq 0$ and γ a pattern. For every $k \geq 0$, let $c_N[k, (\gamma, H_n)]$ denote the number of self-avoiding walks in S_N for which (γ, H_n) occurs at no more than k different steps.

We have already defined a self-avoiding walk in Definition 2.2.3. Now we give a few more definitions which are related to the self-avoiding random loop which will be used in Chapter 4.

Definition 2.3.4 *A **random self-avoiding N-walk** is an uniformly distributed random element of the set of self-avoiding N-walks. (It is a sequence of independent random variables)*

Definition 2.3.5 *Let, $\omega = \{\omega(0), \cdots, \omega(N-1)\}$ be an N-walk. Then, ω is a* ***self-avoiding N-loop*** *if,*

$$\sum_{k=0}^{i} \omega(k) \neq \sum_{k=0}^{j} \omega(k), \forall i \neq j.$$

and $\omega(0) = \omega(N)$. A random self-avoiding N-loop is a uniformly distributed random element of the set of self-avoiding N-loops.

2.4 Connective Constant

Polymer molecules become self-entangled when they are in a solution. This may change the property of the polymer. So, it is quite interesting to know the possible number of configurations of a polymer chain in a solution. Since, c_N gives the number of possible configurations, so finding out its limit as $N \to \infty$ may help us to find out the number of possible configurations as the length of the polymer N increases. In (2.6) we can see that the sequence $\{c_q\}$ is submultiplicative. Using the Lemma 2.2.1, we can ensure that the $\lim_{N\to\infty} c_N^{\frac{1}{N}}$ exists, where this limit is taken as μ and $c_N \geq \mu^N$. This limit μ is known as the **connective constant**. The precise value of μ is not known in any dimensions. Rigorous lower and upper bounds on the connective constant for a cubic lattice, μ_c is given in [20]. The bounds given in table 2.2. The references given in table 2.2 for (a), (b), (c), (d), (e) and (f) are as follows, (a) corresponds to [3], (b) corresponds to [20], (c) corresponds to [11], (d) corresponds to [2] and [10], (e) corresponds to [9] and (f) corresponds to [8]. Nienhuis in [16] showed that for

d	Lower Bound	Estimate	Upper Bound
2	2.620 (a)	2.63815 (d)	2.695 (b)
3	4.572 (c)	4.68390 (c)	4.756 (b)
4	6.742 (c)	6.7720 (c)	6.832 (b)
5	8.828 (c)	8.8386 (e)	8.881 (b)
6	10.874 (c)	10.8788 (e)	10.903 (b)

Table 2.2: Lower and upper bound for μ_c for dimensions 2,3,4,5,6

2-dimensional hexagonal lattice, there is strong evidence from physical arguments, that $\mu = \sqrt{2+\sqrt{2}} \approx 1.847759$. In [1], Alm and Parviainen have used a relation between the hexagonal lattice and the (3.12^2) to improve the bounds for the connective constant, μ, for the hexagonal lattice.

Chapter 3

Pattern Theorem

When a linear polymer is in a solution, it can become self entangled and may undergo a ring closer reaction. Frisch and Wasserman in [7] and Delbruk in [4] conjectured that sufficiently long ring polymers would be knotted with probability one. The validity of Frisch-Wasserman-Delbruk conjecture was established for a lattice model of a polymer by Sumners and Whittington in [21] and independently by Pippenger in [17]. In [22], Whittington has discussed about knotted polymers and N-edge polygons. If p_N is the number of polygons with N edges in Z^3 and p_N^0 is the number of N-edge polygons which are unknotted, then, it can be shown that the ratio $\frac{p_N^0}{p_N}$ goes to zero exponentially rapidly as $N \to \infty$. This means that the probability that a randomly chosen polygon with N-edges is knotted goes to unity exponentially rapidly. Whittington in [22] has examined the methods used in proving this result, and their various extensions.

An interesting statistic regarding patterns is the frequency of occurrence of a particular pattern at the beginning of a self-avoiding walks. In general dimension d, it is an open problem to prove that the fraction of N-step self-avoiding walks that begin with a given pattern converges as N tends to infinity. Kesten in [13] showed that $\lim_{N\to\infty} \frac{c_{N+2}}{c_N}$ = connective constant of the cubic lattice in all dimension, using an argument based on 'Pattern Theorem'. Kesten's Pattern Theorem states that, if a given pattern can possibly occur several times in a self-avoiding walk, then it must occur at least aN times on almost all N-step self-avoiding walks, for some $a > 0$. Now let us state our version of Kesten's Pattern Theorem for the hexagonal lattice.

Theorem 3.0.1 *Let H be a hexagonal ball in the hexagonal lattice and μ be the connective constant for the hexagonal lattice $\mathbb{H}$.*

(a) γ be a pattern as in Definition 2.3.3. Then there exists an $a > 0$ such that

$$\limsup_{N\to\infty}(c_N[aN,(\gamma,H)])^{\frac{1}{N}} < \mu. \tag{3.1}$$

(b) For any proper internal pattern γ, there exists an $a > 0$, such that

$$\limsup_{N\to\infty}(c_N[aN,\gamma])^{\frac{1}{N}} < \mu. \tag{3.2}$$

This theorem has been proved for cubic lattices by Kesten. Our aim is to show that, this theorem still holds when the lattice is a hexagonal lattice.

3.1 Pattern Theorem for Hexagonal Lattice

Kesten's Pattern Theorem for cubic lattices depend on three main lemmas. To show Theorem 3.0.1, we will be following the similar path by checking whether the three lemmas hold for hexagonal lattice structures. The first lemma is about filling up a lattice by a self-avoiding walk and extending a proper internal pattern inside an n-layered hexagonal ball H_n to an $(n+2)$-layered hexagonal ball H_{n+2}.

Lemma 3.1.1 *(a) Let H be a hexagonal ball in $\mathbb{H}$. Then there exists a self-avoiding walk ω, whose endpoints are two of the lattice points of the outermost layer of H, which is entirely contained in H and visits every point of H. Also, the number of steps in ω is one less than the number of points in H.*

(b) Let $\gamma = (\gamma(0), \cdots, \gamma(k))$ be a pattern contained in the n-layered hexagonal ball H_n, whose endpoints are two of the lattice points of the outermost layer of H_n, i.e., $\overline{\gamma}(0)$ and $\overline{\gamma}(n) \in l_n$. Let x and y be two distinct outer points of $l_{n+1} \cup l_{n+2}$. Then there exists a self-avoiding walk ω' with the following properties: Its initial point is x and its last point is y; it is entirely contained in H_{n+2}; there exists a j such that $\overline{\omega'}(j+i) = \overline{\gamma}(i)$ for every $i = 0, \cdots, k$; and $\omega'(i) \in l_{n+1} \cup l_{n+2}$ whenever $i < j$ or $i > j+k$. In particular, (γ, H) occurs at the j-th step of ω' as in definition 2.3.2.

Idea of the proof: We can fill up a hexagonal ball by a self-avoiding walk which visits every lattice point of the hexagonal ball. The way a hexagonal ball can be filled

up is to follow the path of spiral in and spiral out. We can see it from Figure 3.1. Part (a) of Lemma 3.1.1 is clear from Figure 3.1. The pattern in Figure 3.1 suggests

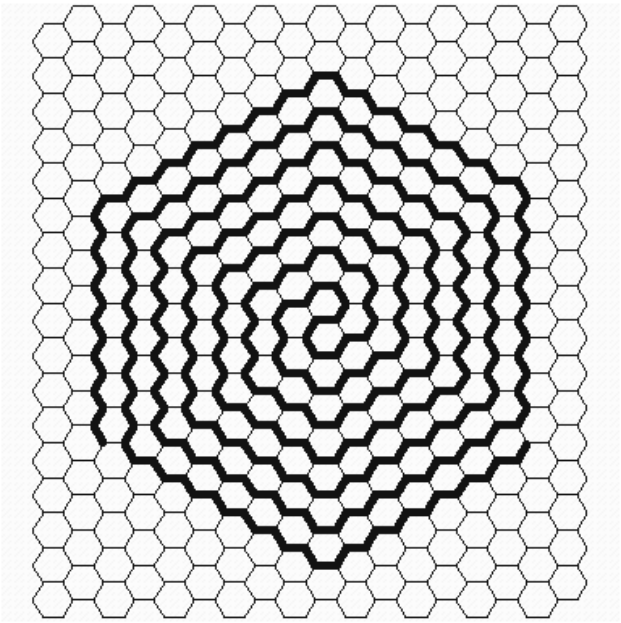


Figure 3.1: Filling up a hexagonal ball

how to fill up a hexagonal ball in general. Part (b) of the lemma can be shown by using part (a) of the lemma. □

Now we are defining some events which depend on how many lattice points are being covered on the lattice structure, by the self-avoiding walk ω. The event E^* occurs at the j-th step of ω if $H_n(j)$ is completely covered by ω. For every $k \geq 1$, we say that the event E_k occurs at the j-th step of ω if at least k points of $H_{n+2}(j)$ are covered by ω. The event $\tilde{E}_k$ occurs at the j-th step of ω if E^* or E_k (or both) occur there. We will be using E to denote any of E^*, E_k or $\tilde{E}_k$.

Let m be a positive integer. We say that the event $E(m)$ occurs at the j-th step of ω if E occurs at the m-th step of the $2m$ step walk $(\omega(j-m), \cdots, \omega(j+m))$. If $j-m<0$ or $j+m>N$, then we will modify the definition: for $j-m<0$, it means E occurs at the j-th step of $(\omega(0), \cdots, \omega(j+m))$. For $j+m>N$, it means E occurs at the m-th step of $(\omega(j-m), \cdots, \omega(N))$. In particular, if $E(m)$ occurs at the j-th step of ω, then E occurs at the j-th step of ω. For every $k \geq 0$, let

$$\begin{aligned} c_N[k,E] &= \#\text{ of self-avoiding walks in } S_N \text{ for which} \\ &\quad E \text{ occurs at no more than } k \text{ different steps} \\ c_N[k,E(m)] &= \#\text{ of self-avoiding walks in } S_N \text{ for which} \\ &\quad E(m) \text{ occurs at no more than } k \text{ different steps.} \end{aligned}$$

$c_N[k,E(m)]$ is the non-increasing function in m for fixed N and k, since occurrences of $E(m)$ are more frequent as m increases.

Theorem 3.0.1 states that certain configurations occur *quite often* except in a small set of walks. We are trying to show that *quite often* a self-avoiding walk fills up a whole hexagonal ball. Lemma 3.1.2 tells us that if the event E occurs on almost all walks, then for some m, $E(m)$ must occur on almost all walks.

Lemma 3.1.2 *If*

$$\liminf_{N\to\infty}(c_N[0,E])^{\frac{1}{N}} < \mu \tag{3.3}$$

then, there exists an $a_1 > 0$ *and an integer* m *such that*

$$\limsup_{N\to\infty}(c_N[a_1N, E(m)])^{\frac{1}{N}} < \mu. \tag{3.4}$$

So it means that, if a self-avoiding walk is likely to fill a hexagonal ball, then it is also likely to fill a hexagonal ball within some bounded number of steps. The proof of Lemma 3.1.2 does not depend on the lattice structure.Thus it is the same for both the cubic lattice structure and the hexagonal lattice structure. This proof of this lemma for cubic lattice is done in [15] and in [13].

Proof: Let us notice that, a path of length greater than N can occur only after the N-th step. So we have, $c_N[0, E] = c_N[0, E(N)]$. Hence we can say, there exists an $\epsilon > 0$ and an integer m, such that,

$$c_m[0, E(m)] < (\mu(1-\epsilon))^m$$

and, since, $\lim_{N\to\infty} c_N^{\frac{1}{N}} = \mu$, we have,

$$c_m < (\mu(1+\epsilon))^m.$$

Let us consider an N-step self-avoiding walk ω, and $M = \lfloor\frac{N}{m}\rfloor$. By defining M, we are dividing the N-step self-avoiding walk into M number of m-length subwalks. So if $E(m)$ occurs at most k times in ω, then $E(m)$ occurs in at most k of the M number

of m-step subwalks $(\omega((i-1)m), \omega((i-1)m+1), \cdots, \omega(im))$, where, $i = 1, .., M$.

There are $c_m[0, E(m)]$ possible choices for m-step subwalk without $E(m)$ occuring, and at most c_m choices for an arbitrary m-step subwalk. If $E(m)$ occurs in j of the M pieces of length m, then, their places can be chosen in $\binom{M}{j}$ ways.

So, we have to count the number of ways in which k or fewer of these subwalks can contain an occurrence of $E(m)$, and also counting the last $(N - Mm)$ steps of ω we have the bound,

$$\begin{aligned} c_N[k, E(m)] &\leq \sum_{j=0}^{k} \binom{M}{j} (c_m)^j (c_m[0, E(m)])^{M-j} c_{N-Mm} \\ &\leq \sum_{j=0}^{k} \binom{M}{j} (\mu(1+\epsilon))^{jm} (\mu(1-\epsilon))^{m(M-j)} c_{N-Mm} \\ &= \mu^{mM} c_{N-Mm} \sum_{j=0}^{k} \binom{M}{j} (1+\epsilon)^{jm} (1-\epsilon)^{Mm-jm} \end{aligned} \tag{3.5}$$

It is sufficient to show that there is a ρ, where $0 < \rho < \frac{1}{2}$ and a $t < 1$ such that,

$$c_N[\rho M, E(m)]^{\frac{1}{M}} < t\mu^m \tag{3.6}$$

for all sufficiently large M, as this gives (3.4) whenever $0 < a_1 < \frac{\rho}{m}$. But if ρ is a small positive number, then,

$$\sum_{j=0}^{\rho M} \binom{M}{j} (1+\epsilon)^{jm} (1-\epsilon)^{Mm-jm} \leq (\rho M + 1) \binom{M}{\rho M} \left(\frac{1+\epsilon}{1-\epsilon}\right)^{\rho M m} (1-\epsilon)^{Mm} \tag{3.7}$$

(since, $\binom{M}{j} \leq \binom{M}{\rho M}$ for $0 < \rho < \frac{1}{2}$, and hence,

$$\sum_{j=0}^{\rho M} \binom{M}{j} \leq (\rho M + 1)\binom{M}{\rho M}.)$$

As, $M \to \infty$, the M-th root of the right hand side of (3.7) converges to

$$\frac{1}{\rho^{\rho}(1-\rho)^{(1-\rho)}} \left(\frac{1+\epsilon}{1-\epsilon}\right)^{\rho m} (1-\epsilon)^{m}$$

which is less than 1 whenever $0 < \rho < \rho_0$, for sufficiently small ρ_0. Combining this with (3.5), we see that (3.6) holds if $0 < \rho < \rho_0$ and M is sufficiently large. □

The next lemma plays a very significant role in Kesten's Pattern Theorem. This lemma says that almost all walks fill some hexagonal ball. The proof of this lemma is done by contradiction.

Lemma 3.1.3 *We have,*

$$\liminf_{N\to\infty} (c_N[0, E^*])^{\frac{1}{N}} < \mu \tag{3.8}$$

Proof: Suppose that the lemma is <u>not</u> true, i.e. assume that, $\liminf_{N\to\infty} (c_N[0, E^*])^{\frac{1}{N}} \geq \mu$. As $c_N[0, E^*]^{\frac{1}{N}} \leq \mu$, so,

$$\lim_{N\to\infty} (c_N[0, E^*])^{\frac{1}{N}} = \mu. \tag{3.9}$$

Let us denote the number of layers of the hexagonal ball by n. So $n = 5$ would mean that the hexagonal ball has 5 layers. We make the following observations.

1. $c_N\left[0, \tilde{E}_k\right]$ is a non-decreasing function of k. $c_N\left[0, \tilde{E}_k\right]$ is the number of N-step self-avoiding walks which do not cover k points of H and do not fill the hexagonal ball and $c_N\left[0, \tilde{E}_{k+1}\right]$ is the number of n-step self-avoiding walk which do not cover $k+1$ points of H and do not fill the hexagonal ball. If C_k denotes the set $c_N\left[0, \tilde{E}_k\right]$ and C_{k+1} denotes the set $c_N\left[0, \tilde{E}_{k+1}\right]$, then, $|C_{k+1}| \geq |C_k|$, and hence we can say that $c_N\left[0, \tilde{E}_k\right]$ is a non-decreasing function of k.

2. If E^* does not occur on a given walk, then $E_{(6n^2+6n+1)}$ cannot occur, where, $(6n^2+6n+1)$ is the number of lattice points of an n-layered hexagonal ball H_n. Hence,

$$c_N[0, E^*] \leq c_N[0, E_{(6n^2+6n+1)}] \leq c_N \tag{3.10}$$

and hence (3.9) and (3.10) implies that,

$$\lim_{N\to\infty} c_N[0, \tilde{E}_{(6n^2+6n+1)}]^{\frac{1}{N}} = \mu. \tag{3.11}$$

3. $c_N[0, \tilde{E}_{(n+4)}] = 0, \forall N \geq n+3$.

The first $(n+4)$ points of any walk which starts from origin, must be in $H_{n+2}(0)$. Therefore we can say that, there exists an K such that $n+4 \leq K < 6n^2+6n+1$ such that

$$\liminf_{N\to\infty} c_N[0, \tilde{E}_K]^{\frac{1}{N}} < \mu \tag{3.12}$$

$$\text{and } \liminf_{N\to\infty} c_N[0, \tilde{E}_{K+1}]^{\frac{1}{N}} = \mu. \tag{3.13}$$

By (3.12) and Lemma 3.1.2 , there exists an $a_1 > 0$ and an integer m such that

$$\limsup_{N\to\infty} c_N[a_1 N, \tilde{E}_K(m)]^{\frac{1}{N}} < \mu. \tag{3.14}$$

Let us define the set of self-avoiding walk,

$$T_N = \left\{\omega \in S_N : \tilde{E}_{K+1} \text{ never occurs, } E_K(m) \text{ occurs at least } a_1 N \text{ times } \right\}. \tag{3.15}$$

We can see that by replacing $E_K(m)$ by $\tilde{E}_K(m)$ in (3.15) does not change anything, since the condition that $\tilde{E}_{K+1}$ never occurs ensures that $E^*(m)$ never occurs. Now suppose that, A denotes the set of walks which satisfy (3.12) and B denotes the set of walks which does not satisfy (3.14), then $T_N = A \setminus B$.

So the cardinality condition of T_N satisfies,

$$|T_N| \geq c_N[0, \tilde{E}_{K+1}] - c_N[a_1 N, \tilde{E}_K(m)] = c_N[0, \tilde{E}_{K+1}][1 - \frac{c_N[a_1 N, \tilde{E}_K(m)]}{c_N[0, \tilde{E}_{K+1}]}] \tag{3.16}$$

and therefore, by (3.13) and (3.14),

$$\lim_{N\to\infty} |T_N|^{\frac{1}{N}} = \mu. \tag{3.17}$$

From (3.17) we can say that the pattern is coming more or less everywhere. Hence there is a number K, such that it is not unusual to find lots of hexagonal balls with

exactly K points occupied and no hexagonal balls with more than K points occupied.

Suppose ω is an N-step self-avoiding walk such that $\tilde{E}_{K+1}$ never occurs on ω and $E_K(m)$ occurs at the $j_1th, \cdots, j_sth$ steps of ω (and perhaps at other steps as well). Suppose in addition that,

$$0 < j_1 - m, j_s + m < N \text{ and } j_l + m < j_{l+1} - m, \forall l = 1, \cdots, s-1, \tag{3.18}$$

$$\text{and } H_{n+2}(j_1), \cdots, H_{n+2}(j_s) \text{ are pairwise disjoint.} \tag{3.19}$$

For $l = 1, \cdots, s$ let

$$\sigma_l = \min\{i : \omega(i) \in H_{n+2}(j_l)\}$$

$$\tau_l = \max\{i : \omega(i) \in H_{n+2}(j_l)\}.$$

Since $E_K(m)$ occurs at the j_lth step and E_{K+1} does not occur at the j_lth step, there must be exactly K points of $H_{n+2}(j_l)$ that are occupied by points of ω and those points must lie between $\omega(j_l - m)$ and $\omega(j_l + m)$ on the walk. Hence, $j_l - m \leq \sigma_l < j_l < \tau_l \leq j_l + m, \forall l$ Consider all possible ways of replacing each subwalk $(\omega(\sigma_l), \cdots, \omega(\tau_l))$ by a subwalk that stays inside $H_{n+2}(j_l)$ and completely covers $H_n(j_l)$. A special feature of a filled hexagonal ball is that, if the hexagonal ball $H_n(j_l)$ is filled between the q^{th} and v^{th} step of ω, where $q < v$, then, a lattice point of $H_n(j_l)$ can never be occupied by ω before its q^{th} or after its v^{th} step, because ω is a self-avoiding walk. So we have

ensured that there are no overlap amongst the sub-walks and also no overlap amongst the hexagonal balls $H_n(j_l)$. So we can do this replacement simultaneously for all the walks in the hexagonal balls. This is true by Lemma 3.1.1.

The result is always a self-avoiding walk ψ on which E^* occurs at least s times, and where length N' satisfies,

$$\begin{aligned} N' &< N + s[6(n+2)^2 + 6(n+2) + 1] \\ \text{i.e., } N' &< N + s[6n^2 + 30n + 37]. \end{aligned} \tag{3.20}$$

Consider all triples (ω, ψ, J), where ω is a self-avoiding walk in T_N; $J = \{j_1, .., j_s\}$ is a subset of $\{1, .., N\}$ such that (3.18) and (3.19) hold, $E_K(m)$ occurs at each j_l in J. $s = \lfloor \delta N \rfloor$, ($\delta$ is small positive number) and ψ is a self-avoiding walk that can be obtained from ω and J by the procedure discussed previously.

Now we shall estimate the number of such triples both from above and below to obtain a contradiction.

If the hexagonal ball $H_{n+2}(j_l)$ intersects another hexagonal ball of $(n+2)$ layers, centered at x, then, $||\omega(j) - x|| \leq 2r_{n+2}$, where r_n is defined as $r_n = \sqrt{1+3n^2}$. Now notice that, $2r_{n+2} < r_{2n+5}$. (Note: $2r_{n+2} = 2\sqrt{1+3(n+2)^2}$ and $r_{2n+5} = \sqrt{1+3(2n+5)^2}$, so

$$\begin{aligned} 2\sqrt{1+3(n+2)^2} &< \sqrt{1+3(2n+5)^2} \\ \Rightarrow 12n^2+48n+52 &< 12n^2+60n+76 \\ \Rightarrow n+2 &> 0 \end{aligned}$$

which is true. Hence, we have, $2r_{n+2} < r_{2n+5}$.)

Therefore, if the hexagonal ball $H_{n+2}(j_l)$ intersects another hexagonal ball of $(n+2)$ layers, then $||\omega(j) - x|| < r_{2n+5}$.

Let us consider $(n+2)$ layered hexagonal balls which satisfies $||\omega(j) - x|| < 2r_{2n+5}$. If we move the centers of those hexagonal balls through the $(2n+5)$-th layer vertex points, and through the lattice points of $(2n+4)$-th layer, $(2n+3)$-rd layer, and so on, we will have an estimate of the number of hexagonal balls which will intersect our original hexagonal ball $H_{n+2}(j_l)$ and will have the property $||\omega(j) - x|| < 2r_{2n+5}$. Let V' = No. of $(n+2)$ layered hexagonal balls which will intersect $H_{n+2}(j_l)$. Then $V' < 6(2n+5)^2 + 6(2n+5) + 1$. The expression on the right hand side is the total number of lattice points of a hexagonal ball with $(2n+5)$ layers. Let

$$V = 6(2n+5)^2 + 6(2n+5) + 1 = 24n^2 + 132n + 156.$$

Therefore, $V' < V$.

The number of such triples is at least the cardinality of T_N times the minimum number of possible choices of J for walks ω in T_N. Let us define $u = \lfloor \frac{a_1 N}{(2m+2)V} \rfloor$. Each ω in T_N contains at least $a_1 N$ occurences of $E_K(m)$ and so we can find $h_1 < \cdots < h_u$, such that

1. $E_K(m)$ occurs at the h_l th step of ω for every $l = 1, \cdots, u$

2. $0 < h_1 - m, h_u + m < N$ and $h_l + m < h_{l+1} - m$ for every $l = 1, \cdots, u-1$

3. The hexagons $H_{n+2}(h_1), .., H_{n+2}(h_u)$ are pairwise disjoint.

Now, any subset of $\{h_1, .., h_u\}$ that has cardinality $\lfloor \delta N \rfloor$ is a possible choice for J. So if we set, $\rho = \frac{a_1}{(2m+2)V}$, then,

$$\text{No. of triples } \geq |T_N| \binom{\rho N - 2}{\lfloor \delta N \rfloor}. \tag{3.21}$$

For an upper bound, consider a triple, (ω, ψ, J).Observe that E^* occurs at least $|J| = [\delta N]$ times on ψ. It may occur more than $|J|$ times because when we are making a change in a hexagonal ball $H_{n+2}(j_l)$, it can produce occurrences of E^* in some of the hexagonal balls with $(n+2)$ layers that intersects $H_{n+2}(j_l)$. Since, E^* never occurs on ω, we infer that E^* no more than $V|J|$ times on ψ. Hence, given ψ,there are atmost $\binom{V[\delta N]}{[\delta N]}$ possibilities for the locations of the hexagons $H_{n+2}(j_l), l = 1, ..|J|$. Given ψ and the locations of these $|J|$ hexagons, each hexagon $H_{n+2}(j_l)$ determines a subwalk of ψ that replaced some subwalk of ω.

Since each of the replaced subwalks of ω had length $2m$ or less, there are at most $(\sum_{i=0}^{2m} c_i)^{\delta N}$ possibilities for ω if we know both ψ and the locations of the $|J|$ hexagonal balls.

Finally, if we know ω and the locations of the hexagonal balls, then J is uniquely determined. Since, if we define, $Z = (\sum_{i=0}^{2m} c_i)$, then using $\binom{V\delta N}{\delta N} \leq 2^{V\delta N}$ and (3.20) we see that,

$$\text{No. of triples } \leq 2^{V\delta N} Z^{\delta N} C \tag{3.22}$$

where, $C = \sum_{i=0}^{g(n,N)\delta N} c_i$ and $g(n,N) = N + (6n^2 + 30n + 37)$. Combining (3.21) and (3.22), taking N-th root and letting $N \to \infty$, we get by (3.17),

$$\mu\rho^\rho / \left\{\delta^\delta (\rho - \delta)^{\rho-\delta}\right\} \leq 2^{V\delta} \mu^{1+(6n^2+30n+37)\delta} Z^\delta. \tag{3.23}$$

Let $Y = 2^V \mu^{1+(6n^2+30n+37)} Z, t = \delta/\rho,$. Then (3.23) is equivalent to ,

$$1 \leq (t^t (1-t)^{1-t} Y^t)^\rho. \tag{3.24}$$

Consider

$$f(t) = t^t (1-t)^{1-t} Y^t. \tag{3.25}$$

We have, $f(t) < 1$ for sufficiently small $t > 0$, as $\lim_{t \downarrow 0} f(t) = 1$ and $\lim_{t \downarrow 0} f'(t) = -\infty$. Hence we get $f(t)^\rho < 1$ and thus contradicting (3.24) which says that $1 \leq [f(t)]^\rho$.

Hence $\liminf_{N\to\infty} (c_N[0, E^*])^{\frac{1}{N}} < \mu$ is true. □

Now we will prove Theorem 3.0.1, which is Kesten's Pattern theorem for hexagonal lattice.

Proof of Theorem 3.0.1: Let us assume that the hexagonal ball H in the statement of the theorem is

$$H_n = \{x \in \mathbb{H} : |x| \leq r_n\}.$$

Let us suppose that the theorem is <u>not</u> true. Then, for every $a > 0$,

$$\limsup_{N\to\infty}(c_N[aN, (\gamma, H)])^{\frac{1}{N}} = \mu. \tag{3.26}$$

Now we define an event E^{**}. The event E^{**} *occurs at the j-th step of ω if the hexagonal ball H_{n+2} is completely covered by ω.* By Lemma 3.1.2 and Lemma 3.1.3, we can say, there exists $a' > 0$ and m' such that,

$$\limsup_{N\to\infty}(c_N[a'N, E^{**}(m')])^{\frac{1}{N}} < \mu. \tag{3.27}$$

Let $a > 0$ be a small unspecified number, and let $\mathcal{T}_N$ be defined as the following set of walks,

$$\begin{aligned}\mathcal{T}_N &= \{\omega \in S_N : (\gamma, H_n) \text{ occurs at most } aN \text{ times on } \omega;\\ &\qquad E^{**}(m') \text{ occurs at least } a'N \text{ times }\}.\end{aligned}$$

Hence, the cardinality of $\mathcal{T}_N$ satisfies,

$$|\mathcal{T}_N| \geq c_N[aN, (\gamma, H_n)] - c_N[a'N, E^{**}(m')].$$

So, by (3.26) and (3.27), we have,

$$\lim_{N\to\infty} |\mathcal{T}_N|^{\frac{1}{N}} = \mu. \tag{3.28}$$

Let δ be a small positive number. Consider all triples (ω, u, J), such that, ω is in $\mathcal{T}_N$; $J = \{j_1, \cdots, j_s\}$ is a subset of $\{1, \cdots, N\}$ such that $E^{**}(m')$ occurs at each j_l. ((3.18) of Lemma 3.1.3 holds here when we are replacing m by m'.) Also we have, $s = \lfloor \delta N \rfloor$. u is a self-avoiding walk obtained by replacing the occurrence of $E^{**}(m')$ at each j_l by an occurrence of (γ, H_n), similar to the method used in the proof of Lemma 3.1.3. We will define similar to Lemma 3.1.2 for $l = 1, \cdots, s$, let,

$$\sigma_l = \min\{i : \omega(i) \in H_{n+2}(j_l)\}$$

$$\tau_l = \max\{i : \omega(i) \in H_{n+2}(j_l)\}.$$

We can say that the occurrences of $E^{**}(m')$ makes sure that (3.19) holds. Making a similar argument as in (3.21), we have,

$$\text{No. of triples } \geq |\mathcal{T}_N| \binom{\rho N - 2}{\delta N} \tag{3.29}$$

where $\rho = \frac{a'}{(2m'+2)}$. For the upper bound we use the fact that u has almost $aN + 2m'V\delta N$ occurrences of (P, H_n). This allows for

i) at most aN occurrences of (γ, H_n) on ω.

ii) the possibility that changing a single occurrence of $E^{**}(m')$ to a (P, H_n) may create several other occurrences of (P, H_n) either by creating additional occurrences of γ or by vacating sites of other hexagonal balls.

Also note that u has at most N steps. Therefore to the analogue of (3.22), here we have,

$$\text{No. of triples } \leq 2^{aN+2m'V\delta N} Z'^{\delta N} D \tag{3.30}$$

where, $D = \sum_{i=0}^{N} c_i$ and $Z' = \sum_{i=0}^{2m'} c_i$. We combine (3.29) and (3.30) and put $a = \delta$, taking N-th roots, and let $N \to \infty$, by (3.28) we get,

$$\mu \frac{\rho^\rho}{\delta^\delta (\rho - \delta)^{(\rho-\delta)}} \leq 2^{aN+2m'V\delta N} Z'^{\delta N} \mu. \tag{3.31}$$

Similar to the proof of Lemma 3.1.2, this leads to a contradiction for sufficiently small δ, and hence the theorem is proved. □

3.2 Application of Pattern Theorem

Linear polymers become self-entangled when they move in solution.These entanglements are interesting to polymer physicists. If the polymer is self-entangled, then

the entanglement can be preserved in the crystallization process producing a defect or fault in the crystal. Also, when the polymers become self-entangled, the physical and chemical properties of the polymer solution may change. Let $P(N,\gamma)$ denote the probability that an N-step self-avoiding walk contains the pattern γ. Then similar to the theorem about an knotted N-gon in [22], we have the following theorem about patterns.

Theorem 3.2.1 *Let γ be a proper internal pattern on an N-step self-avoiding walk on a hexagonal lattice. Then*

$$\lim_{N\to\infty} P(N,\gamma) = 1. \tag{3.32}$$

Proof: Let us suppose that,

$$\begin{aligned} c^0_{N,\gamma} &= \#\text{ of } N\text{-step self-avoiding walk without } \gamma \\ c_N &= \#\text{ of } N\text{-step self-avoiding walk.} \end{aligned}$$

By concatenation property and by sub-additivity Lemma 2.2.1, we can say that $\lim_{N\to\infty} \frac{\ln c^0_{N,\gamma}}{N}$ and $\lim_{N\to\infty} \frac{\ln c_N}{N}$ exists, and suppose they are,

$$\lim_{N\to\infty} \frac{\ln c^0_{N,\gamma}}{N} = \kappa_0 \tag{3.33}$$

$$\lim_{N\to\infty} \frac{\ln c_N}{N} = \kappa. \tag{3.34}$$

From Kesten's Pattern Theorem 3.0.1, we get that,

$$\begin{aligned} \limsup_{N\to\infty} \frac{\ln c^0_{N,\gamma}}{N} &< \kappa \\ \Rightarrow \kappa_0 &< \kappa. \end{aligned} \tag{3.35}$$

From (3.34) we get,

$$\begin{aligned} \lim_{N\to\infty} \frac{\ln c_N}{N} &= \kappa \\ \Leftrightarrow \lim_{N\to\infty} \left(\frac{\ln c_N}{N} - \kappa \right) &= 0 \\ \Leftrightarrow \lim_{N\to\infty} \left(\frac{\ln c_N - N\kappa}{N} \right) &= 0 \\ \Leftrightarrow \ln c_N - N\kappa &= o(N) \\ \Leftrightarrow \ln c_N &= N\kappa + o(N) \\ \Leftrightarrow c_N &= e^{N\kappa + o(N)}. \end{aligned} \tag{3.36}$$

Similarly $c^0_{N,\gamma} = e^{N\kappa_0 + o(N)}$. So, $\frac{c^0_{N,\gamma}}{c_N} = e^{N(\kappa_0 - \kappa) + o(N)} \to 0$ as $N \to \infty$. Now, as, $P(N,\gamma)$ is the probability that an N-step self-avoiding walk contains the pattern γ, and $\kappa - \kappa_0 > 0$ by (3.35), hence, we have,

$$P(N,\gamma) = 1 - \frac{c^0_{N,\gamma}}{c_N}. \tag{3.37}$$

Now, taking $N \to \infty$ in (3.37), and since, $\kappa - \kappa_0 > 0$, we have,

$$\lim_{N\to\infty} P(N, \gamma) = 1. \tag{3.38}$$

□

So this theorem shows that the probability of occurrence of a pattern in a self-avoiding walk is a sure event as the length of the walk increases.

3.3 Discussions

From the proof of Kesten's Pattern theorem for the hexagonal lattice, we can see that, it is basically similar to Kesten's Pattern theorem for cubic lattices. Here we have followed a similar path. We have used the three lemmas given for cubic lattice and changed only those parts which are really dependent on the lattice structure. Lemma 3.1.2 does not depend on lattice structure, hence no change has been done there. But for Lemma 3.1.1, Lemma 3.1.3 and the main proof and statement of Theorem 3.0.1, we have used some properties of the hexagonal lattice and changed some parts of the proof accordingly.

In [1], Alm and Parviainen give improved bounds for the connective constant of a hexagonal lattice μ. The lower bound is determined by using Kesten's method of irreducible bridges and by determining generating functions for bridges on one dimensional lattices. In [13], Kesten has used a method to find the lower bound

for the connective constant for cubic lattice depending upon *irreducible bridges*. We will now describe some definitions and ideas discussed by Kesten in [13] for finding upper and lower bounds of the connective constant of the cubic lattice and some improvisation made by Alm and Parviainen in [1] for finding upper and lower bound for the connective constant μ of the hexagonal lattice.

Definition 3.3.1 *Let us denote the coordinates of a lattice point of a self-avoiding walk ω by $(\omega(x_i), \omega(y_i))$. A **bridge** of length N is a self-avoiding walk, such that,*

$$\omega(y_0) < \omega(y_i) \leq \omega(y_N), i = 1, \cdots, N-1$$

*An **irreducible bridge** is a bridge that cannot be decomposed into two bridges.*

Define, $b_N = \#$ of bridges of length N and $a_N = \#$ of irreducible bridges of length N. Kesten showed that, for the connective constant of the cubic lattice,

$$\lim_{N\to\infty} b_N^{\frac{1}{N}} = \lim_{N\to\infty} a_N^{\frac{1}{N}} = \lim_{N\to\infty} c_N^{\frac{1}{N}} = \mu$$

i.e. the connective constant for bridges and irreducible bridges are the same for the self-avoiding walk. We can think of the N-step self-avoiding walks, the bridges and the irreducible bridges as sequences. Sometimes the behavior of a sequence can be understood by its generating function. The generating function for the sequence $\{c_N\}$

of N-step self-avoiding walk, can be defined as,

$$C(x) = \sum_{N=0}^{\infty} c_N x^N, c_0 = 1. \tag{3.39}$$

Similar to (3.39), we can define generating functions of bridges and irreducible bridges. Suppose we denote the generating function of bridges by $B(x)$ and the generating function of irreducible bridges of $A(x)$. Then, in [1] it is shown that, if

$$B(x) = \sum_{N=0}^{\infty} b_N x^N, b_0 = 1 \tag{3.40}$$

$$A(x) = \sum_{N=0}^{\infty} a_N x^N, a_0 = 1, \tag{3.41}$$

then the relation between $B(x)$ and $A(x)$ is,

$$B(x) = \frac{1}{1 - A(x)}. \tag{3.42}$$

The radius of convergence of the series $A(x)$ is, μ^{-1}. Alm and Janson earlier showed that it is theoretically possible to calculate $B_N(x)$ and hence we can have $A_N(x)$ by (3.42). In [1], Alm and Parviainen have used a similar method to calculate the generating functions for bridges and irreducible bridges for hexagonal lattice structures. For this they have used a different embedding of the hexagonal lattice as shown in Figure 3.2. On this embedding (Figure 3.2) of hexagonal lattice, bridges, irreducible bridges can be defined similar to that of a cubic lattice. The best upper and lower

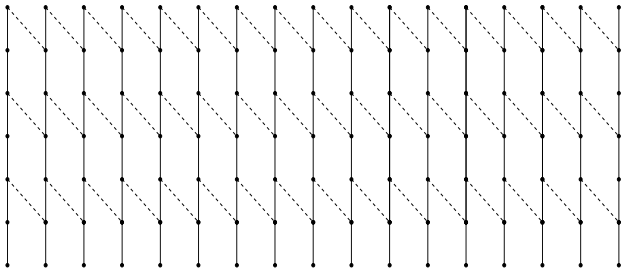


Figure 3.2: A different embedding of hexagonal lattice

bounds found by Alm and Parviainen in [1] is,

$$1.833009764 < \mu < 1.868832$$

where the actual conjectured value of the connective constant of the hexagonal lattice, $\mu = \sqrt{2+\sqrt{2}} \approx 1.847759$.

Chapter 4

Self-Avoiding Random Loops

In Chapter 1, we defined self-avoiding walks, patterns, some properties of self-avoiding walks on hexagonal lattice structures. In this part we will look at self-avoiding random loops. In [6], Dubins *et al.* described *a random loop, or polygon* as a *simple random walk whose trajectory is a simple closed Jordan curve.* It was shown in [6] that the probability that a random N-step loop contains the point $(\frac{1}{2}, \frac{1}{2})$ in the interior of the loop is $\frac{1}{2} - \frac{1}{N}$. In this chapter, we will extend this result to hexagonal lattices. Let us consider a self-avoiding N-loop $\alpha = \{\alpha(0), \cdots, \alpha(N-1)\}$. The points $\alpha(0), \cdots, \alpha(N-1)$ together with the unit line segments joining $\alpha(j)$ to $\alpha(j+1)$, for $j = 0, \cdots, (N-1)$, forms a simple closed Jordan curve J in the plane with vertices $\alpha(0), .., \alpha(N-1)$. A Jordan curve partitions the plane into an inside and an outside region. It is of interest to know what would be the probability that a point (x, y) on the plane is inside, outside or on the Jordan curve J and what would

be the probability that the two points (x, y) and $(x, -y)$ on the plane would both be inside, outside or on the curve. In the next two theorems we will find the probability of the points $(\frac{1}{2}, \frac{1}{2})$ is inside the Jordan curve and the probability of the point $(\frac{1}{2}, \frac{1}{2})$ and $(\frac{1}{2}, -\frac{1}{2})$ are both inside the Jordan curve when the lattice is a hexagonal lattice.

4.1 Encircling the points $(\frac{1}{2}, \frac{1}{2})$ and $(\frac{1}{2}, -\frac{1}{2})$

In this section we will calculate the probability of a self-avoiding random loop to encircle the point $(\frac{1}{2}, \frac{1}{2})$ and both the points $(\frac{1}{2}, \frac{1}{2})$ and $(\frac{1}{2}, -\frac{1}{2})$. We modify the method of Dubins *et al.* in [6] for the hexagonal lattice. We now state and prove the version for the hexagonal lattice structure.

Theorem 4.1.1 *Let $\alpha = \{\alpha(0), \cdots, \alpha(N-1)\}$ be a random self-avoiding N-loop in a hexagonal lattice tracing a Jordan curve J with the origin as one of its vertices. Let us consider two points $A = \left(\frac{1}{2}, \frac{1}{2}\right)$, and $B = \left(\frac{1}{2}, -\frac{1}{2}\right)$. Then,*

a) the probability that the point A is inside the random self-avoiding N-loop is,

$$P\left(A \in J\right) = \frac{1}{2} - \frac{1}{N}; \tag{4.1}$$

b) the probability that the points A and B are both inside the random self-avoiding N-loop is,

$$P\left(A \text{ and } B \text{ are inside } J\right) = \frac{1}{6} - \frac{1}{N}. \tag{4.2}$$

Proof : For a self-avoiding random N-loop α on a hexagonal lattice. N will be even. J consists of the points $\alpha(0), \cdots, \alpha(N-1)$ and the line segements joining $\alpha(k)$ and $\alpha(k+1)$ for $k = 0, \cdots, N-1$. Each $\alpha(k)$ is a vertex of J. At each vertex point, the angle between two adjacent sides is either 120^o or 240^o. Let

$$\begin{aligned} a &= \#\text{ of } 120^o \text{ angles} \\ \text{and } b &= \#\text{ of } 240^o \text{ angles.} \end{aligned}$$

Then

$$N = a + b. \tag{4.3}$$

We have to consider all possible random self-avoiding N-loop which can be drawn in such a way that the origin is a vertex of the loop. This can be done in the following way. We will cyclically permute the trajectory of the vertices to $\overline{\alpha}(k) - \overline{\alpha}(k), \overline{\alpha}(k+1) - \overline{\alpha}(k), \cdots, \overline{\alpha}(k+N) - \overline{\alpha}(k)$ for $k = 0, 1, \cdots, N-1,$ where $\overline{\alpha}(N+i) = \overline{\alpha}(i)$. This way we will be constructing the N Jordan curves $J_0, J_1, \cdots, J_{N-1}$. If we rotate each of the Jordan curve J_i, for $i = 0, \cdots, N-1$, through, $0^o, 120^o$ and 240^o, then we will get $3N$ Jordan curves, which would be the total number of possible Jordan curves which would have origin as a vertex. Some of the Jordan curves may be identical, but our J maybe any of these $3N$ Jordan curves with equal probability. Now we try to do part (a) of the theorem. We will try to calculate the fraction p_1 of these Jordan curves which will contain the point $\left(\frac{1}{2}, \frac{1}{2}\right)$, and for part (b), we will try to calculate

the fraction p_2 of these Jordan curves which will contain both the points $\left(\frac{1}{2}, \frac{1}{2}\right)$ and $\left(\frac{1}{2}, -\frac{1}{2}\right)$. From properties of external angle of a polygon, we have,

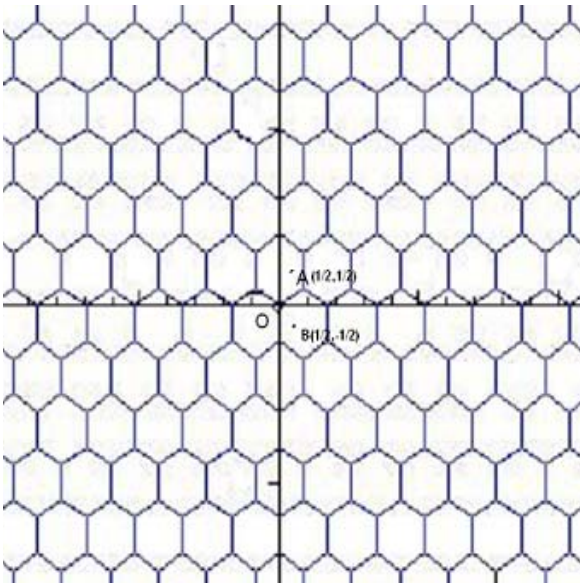


Figure 4.1: Encircling the points A and B

$$\begin{aligned} a\frac{\pi}{3} - b\frac{\pi}{3} &= 2\pi \\ \Rightarrow a - b &= 6. \end{aligned} \tag{4.4}$$

Solving (4.3) and (4.4) for a and b in terms of N, we get,

$$a = \frac{N+6}{2} \tag{4.5}$$

$$b = \frac{N-6}{2}. \tag{4.6}$$

a) Now, suppose that at the vertex $\alpha(k)$ of J, the angle is 120^o. Then, exactly one of the three rotations of J_i will contain the point $\left(\frac{1}{2}, \frac{1}{2}\right)$. If at the vertex $\alpha(k)$ of J, the angle is 240^o, then for exactly two of the three rotations of J will contain the point $\left(\frac{1}{2}, \frac{1}{2}\right)$. So, we have the fraction p_1 as,

$$p_1 = \frac{a + 2b}{3N}. \tag{4.7}$$

Using, (4.5) and (4.6) in (4.7), we get,

$$\begin{aligned} p_1 &= \frac{a + 2b}{3N} \\ &= \frac{\frac{N+6}{2} + 2\frac{N-6}{2}}{3N} \\ &= \frac{1}{2} - \frac{1}{N}. \end{aligned}$$

Now we show part (b) of the theorem.

b) Similar to part (a), suppose that at the vertex $\alpha(k)$ of J, the angle is 120^o. Then, none of the three rotations of J_i will contain the points A and B. If at the vertex $\alpha(k)$ of J, the angle is 240^o, then for exactly one of the three rotations of J will contain the points A and B. So, we have the fraction p_2 as,

$$p_2 = \frac{b}{3N}. \tag{4.8}$$

Using (4.6) in (4.8)

$$p_2 = \frac{b}{3N} = \frac{\frac{N-6}{2}}{3N} = \frac{1}{6} - \frac{1}{N}.$$

Hence, we have proved Theorem 4.1.1. □

4.2 Related Results and Discussions

We can see that it is not so difficult to find the probability that an N-step self-avoiding loop on a hexagonal lattice encircles the point $\left(\frac{1}{2}, \frac{1}{2}\right)$. In [6], it has been conjectured that, whenever x and y are both non-integers on a square lattice, then, $\lim_{N\to\infty} P_N\left((x,y) \in N\text{-step self-avoiding loop }\right) = \frac{1}{2}$. But it is not easy to prove this result even for $(x,y) = \left(\frac{3}{2}, \frac{1}{2}\right)$. So, Dubins *et al.* have used simulations for the point $\left(\frac{3}{2}, \frac{1}{2}\right)$ in [6].

Bibliography

[1] S.E. Alm, R. Parviainen. Bounds for the Connective Constant of the Hexagonal Lattice. *Journal of Physics A: Mathematical and General* **37**, (2004), issue 3, pp. 549-560.

[2] A.R. Conway, I.G. Enting, A.J. Guttman. Algebraic Techniques for Enumerating Self-Avoiding Walks on the Square Lattice. *Journal of Physics A: Mathematical and General* **26**, (1993), pp. 1519-1534.

[3] A.R. Conway, A.J. Guttmann. Lower Bound on the Connective Constant for Square Lattice Self-Avoiding Walks. *Journal of Physics A: Mathematical and General* **26**, (1993), pp. 3719-3724.

[4] M. Delbruck. Mathematical Problems in the Biological Sciences. *American Mathematical Society*, Providence, RI, (1962), pp. 55.

[5] M. Doi. *Introduction to Polymer Physics*. Claredon Press, Oxford, (1996).

[6] L.E. Dubins, A. Orlitsky, J.A. Reeds, L.A. Shepp. Self-Avoiding Random Loops. *IEEE Transactions on Information Theory*, vol. **34**, no. 6, (1988), pp. 1509-1516.

[7] H.L. Frisch, E. Wasserman. Chemical Topology. *Journal of the American Chemical Society* **83**, (1968), pp. 3789-3795.

[8] A.J. Guttmann. On the Zero-Field Susceptibility in the $d = 4$, $n = 0$ Limit: Analysing for confluent Logarithmic Singularities. *Journal of Physics A: Mathematical and General* **11**, (1978), pp. L103-L106.

[9] A.J. Guttmann. Correction to Scaling Exponents and Critical Properties of the n-vector Model with Dimensionality > 4. *Journal of Physics A: Mathematical and General* **14**, (1981), pp. 233-239.

[10] A.J. Guttman, I.G. Enting. The Size and Number of Rings on the Square Lattice. *Journal of Physics A: Mathematical and General* **21**, (1988), pp. L165-L172.

[11] T. Hara, G. Slade, A.D. Sokal. New Lower Bounds on the Self-Avoiding-Walk Connective Constant. *Journal of Statistical Physics*, (1993), pp. 479-517.

[12] G.H. Hardy, S. Ramanujan. Asymptotic Formulae in Combinatory Analysis. *Proceedings of the London Mathematical Society* **17**, (1918), pp. 75-115.

[13] H. Kesten. On the Number of Self-Avoiding Walks. *Journal Of Mathematical Physics*, vol. **4**, no. 7, (July 1963), pp. 960-969.

[14] G.F. Lawler. *Intersections of Random Walks*. Birkhäuser, (1991).

[15] N. Madras, G. Slade. *The Self-Avoiding Random Walk* . Birkhäuser, (1996).

[16] B. Nienhuis. Critical Behavior of Two-dimensional Spin Models and Charge Asymmetry in the Coulomb Gas. *Journal of Statistical Physics* **34**, (1984), pp.731-761.

[17] N. Pippenger. Knots in Random Walks. *Disc. Appl. Math.* **25**, (1989), pp. 273-278.

[18] M. Rubenstein, R.C. Colby. *Polymer Physics*. Oxford University Press, (2004).

[19] J. Rudnick, G. Gaspari. *Elements of the Random Walk, An Introduction for Advanced Students and Researchers*. Cambridge University Press, (2004).

[20] G. Slade. Self-Avoiding Walks. *The Mathematical Intelligencer*, vol. **16**, no. 1, (1994), pp.29-35.

[21] D. W. Sumners, S. G. Whittington. Knots in Self-Avoiding Walks. *Journal of Physics A: Mathematical and General* **21**, (1988), pp. 1689-1694.

[22] S.G. Whittington. Topology of Polymers. *Proceedings of Symposia in Applied Mathematics*, vol. **45**, (1992), pp. 73-95.

Appendix A

Equivalence of two definitions of layers of a hexagonal ball

It can be easily shown that the points in the n-th layer as defined by definition 2.1.2 are either of the distance $n\sqrt{3}$ or $\sqrt{1+(n\sqrt{3})^2} = r_n$ from the center of the hexagonal ball. We can see that the points of the $(n+1)$-th layer l_{n+1} are either of distance $(n+1)\sqrt{3}$ or $\sqrt{1+((n+1)\sqrt{3})^2} = r_{n+1}$. As both these numbers are greater than r_n, the equivalence with definition 2.1.2 and equation (2.2) follows.

Appendix B

Spanning a hexagonal lattice

The proof of (2.4) follows by induction. First notice that for the origins of type (a) in Figure (2.5), the 3 hexagons adjacent to the origin have centers $-\vec{e_1}$, $-\vec{e_2}$ and $\vec{e_1}+\vec{e_2}$ respectively, which are of the form (2.4) with $(m,n) = (1,-1),(0,0)$ and $(1,0)$ respectively. Similarly for origins of type (b) in figure (2.5), the 3 hexagons adjacent to the origin are with centers of the form (2.4) with (m,n) satisfying $m,n \in \{-1,0,1\}$. Now, let us assume the origin is of type (a) and prove the result; type (b) will follow similarly.

Call all the hexagons adjacent to the origin (hexagons having the origin as one of their vertices) as hexagons of stage 1, all the hexagons adjacent to (sharing at least one side with) hexagons of stage 1 but not belonging to stage 1 as stage 2, all hexagons adjacent to hexagons of stage 2 but not belonging to stages 1 or 2 as stage 3, and so on. In general, we define stage $(k+1)$ as the collection of all the hexagons

adjacent to the hexagons of stage k but not belonging to stages 1 to k. So, a layer will overlap with a stage if H_0 is shifted to the origin. We have shown that all the hexagons in stage 1 satisfy (2.4). Now, suppose that all the hexagons in stages k or below satisfy (2.4). Notice now that for any hexagon with center $\vec{a}$, its adjacent hexagons will have centers $\vec{a} + l_1(\vec{e_1} + 2\vec{e_2}) + l_2(2\vec{e_1} + \vec{e_2})$, where $l_1,\ l_2 \in \{-1, 0, 1\}$. This implies that the hexagons in stage $(k+1)$ have centers of the form $m(\vec{e_1}+2\vec{e_2})+ n(2\vec{e_1}+\vec{e_2})-\vec{e_2}+l_1(\vec{e_1}+2\vec{e_2})+l_2(2\vec{e_1}+\vec{e_2}) =(m+l_1)(\vec{e_1}+2\vec{e_2})+(n+l_2)(2\vec{e_1}+\vec{e_2})-\vec{e_2}$, which is again of the form given by (2.4). This completes the induction.

Appendix C

MAPLE codes for generating c_N for different N

The following program has been used to find the values of c_N for different values of N which are showed in table 2.1. This program checks through each of the 3^N walks and see which one is self-avoiding by means of a function p defined in the program.We have given the value for $N = 12$ below. cn gives the value of c_N for $N = 12$. As the number of steps N increases, the time for calculation is also increasing. The program needs to be restarted for each choice of n, which represents N in the program.

```
> restart:

> n:=12;

                        n := 12

> alpha:=array(1..n):w:=exp(I*Pi/3):
```

```
> p:=1:for i from 1 to n

  do for j from i+1 to n

  do h:=sum((-1)^(j-k)*w^(alpha[k]),k=i..j):

  p:=p*h:od:od;

> A:=array(1..3^n):A[1]:=[seq(0,i=1..n)]:

  for k from 0 to n-1

  do for j from 1 to 3^k

  do A[3^k+j]:=A[j]: A[2*3^k+j]:=A[j]: A[3^k+j][n-k]:=1:

  A[2*3^k+j][n-k]:=2: od:od:

> c[n]:=0: for i from 1 to 3^n

  do alpha:=A[i]:

  if p<>0 then print(alpha):

  c[n]:=c[n]+1:fi:od:

> print(c[n]=c[n]);

                cn = 4416
```