FIELD DRIVEN TRANSLOCATION OF A POLYMER INTO A CIRCULAR CAVITY :A TWO–DIMENSIONAL MONTE CARLO SIMULATION STUDY

By

Fikre Jida

SUBMITTED IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE DEGREE OF
MASTER OF SCIENCE IN PHYSICS
AT
ADDIS ABABA UNIVERSITY
ADDIS ABABA, ETHIOPIA
JUNE 2013

ADDIS ABABA UNIVERSITY

DEPARTMENT OF

PHYSICS

Supervisor: _____

Dr. Tatek Yergou

Examiners: _____

Dr.Mulugeta Bekele

_____

Dr.Mesfin Tsige

ADDIS ABABA UNIVERSITY

Date: **June 2013**

Author: **Fikre Jida**

Title: **FIELD DRIVEN TRANSLOCATION OF A POLYMER INTO A CIRCULAR CAVITY :A TWO–DIMENSIONAL MONTE CARLO SIMULATION STUDY**

Department: **Physics**

Degree: **M.Sc.** Convocation: **June** Year: **2013**

Permission is herewith granted to Addis Ababa University to circulate and to have copied for non-commercial purposes, at its discretion, the above title upon the request of individuals or institutions.

Signature of Author

Table of Contents

List of Figures

Abstract

In this thesis the linear polymer transported into a circular cavity hole is simulated. We have used the way of Monte Carlo approach in the presence of the applied external field to study polymer translocation into cavity hole using the 2D fluctuation bond model with single–segment Monte Carlo moves. While an external field is applied we analyze the translocation and concentrate on the translocation time into cavity hole as function of a polymer chain sizes. However there are other influences on forced translocation i.e the field strength,the width of cavity wall and the attractive interaction of the monomers and cavity hole, here we examined only the influence of the length of the chain N on the forced translocation time.The major effect of superimposed monomers number on polymer translocation has been proved. As our main result we found that a crossover scaling for translocation time τ with chain length $\tau \sim N^{1+\nu}$ where ν is the Flory exponent.And the polymer escape time τ is directly proportional with the length of polymer N.

Acknowledgements

First of all, I would like to thank the almighty God who made it possible,to begin and finish this work succesfully. It also gives me a great pleasure to express my gratitude to all persons who have helped and encouraged me in the process of writing this material.
Especially my advisor and instructor Dr.Tatek Yergou I do not have adequate words to express my feelings of gratitude for his many suggestions and continuous support and friendly approach through out this research.His tireless follow up and consistent guidance service for the main possible roots of preparing the material will be in my memory forever. I am very grateful once again to him for all the things that he has done for me.
My acknowledgement extended to my friend Tigst Tajune , Kifle Lemma , my sister Bezash Bekele,Deninesh Yilma , Martha Mersha,my brother Nigusie Jida,Sodo Buee Wereda Administration and Sodo Buee preparatory school principal and the staff members those who are playing a great role for my successful begin and finish .
Finally, I would like to express my sincere thank to Anley Gesese, Solomon Negash ,Tolasa Adugna and Berhanu Aragie for all thier patient support.

Chapter 1

Introduction to polymer physics

In our everyday experience we are constantly in contact with synthetic polymers like plastics,rubbers,gels etc., without mentioning the fundamental role for existence of all life beings played by biopolymers like DNA (Deoxyribonucleicacid),RNA(Ribonucleicacid),protien and viruses. However, the origins of today's polymer industry commonly are accepted as being in the nineteenth century when importrant discoveries were made concerning the modification of certain natural polymer.This is a beautiful starting point to the subject polymer physics[1]. A polymer is chemical compuond or mixture of compounds consisting of repeating structural units created through a process of polymerization . The term derives from ancient Greek word (polus, meaning "many,much") and (meros , meaning "parts").The repeating structural units of ploymer are called monomers.And they are jointed together via covalent bonds. The longest synthetic chains created contains about 10^6 monomers while biopolymers arrive up to 10^{10} (ten billions)of monomers.Macromolecules with less than 100 monomers are too short to sustain the properties of polymers and are not classified as such[2][3]. Based on the species of the monomers that used to make macromolecules(polymer) the polymer can be classified as homopolymer is polymer drived from one species of monomer. And the chemical structure of a polymer usually is represented by that of repeat unit enclosed by bracket. Thus the hypothetica homopolymer(—A—A—A—A—A—) is represented by $(—A—)_n$,where n is

the numbers of repeat units linked together to form macromolecule and hetropolymer is a polymer derived from diffrent species of monomer.And the chemical structure of a polymer usually is represented by that of repeat unit enclosed by bracket.Hence one of hetropolymers is given by (—B—A—B—A—B—A—B—) is represented by $(—B—A—B—)_{n+m}$ where n and m are the numbers of repeat units linked together to form macromolecule[1]. The simplest possible polymer model is presented by ideal chain,corresponding to a simple random walk. Experimental approaches /methods/, helped the mathematical modeling of polymers and even a better understanding of the properties of polymers. Based on thier architecture/shape/,polymers can be classified as linear, brached and cross–linked polymer one as shown in the (fig.1.1). Here, we will focuse on a linear polymers architecture constructed from individual monomeric units they may not be identical.Hence the aim of this section is to introduce the basic concepts of polymer and polymer physics. This leads us the summary of of the static properties for ideal and real polymer chains.

Figure 1.1: Some examples of polymer architectures /shapes/.

1.1 Static properties of polymers

Models of polymer chains are split into two types "ideal" models and "real" models.Ideal chain models assume that there are no interactions between chain monomers. Our computation in this section are based on freely–jointed chain model which is the simplest model describe a polymer. Flexible polymers can take up an enormours number configurations by the rotations of chemical bonds. The shape of polymers can therefore only be usefully described statistically.In this section we will describe statistical properties of a single polymer in the equilibrium sate.

1.1.1 Ideal polymer chains

To study the statistical properties of flexible polymer,let us start a very simple model a chain consisting of N links each of lenght b able to point in any direction independently of each other such a model is called freely jointed chain. The conformation of freely jointed chain is represented by a set of $N+1$ position vector $\overrightarrow{R_i}$(i=0,...,N) or by set of bond vectors $\overrightarrow{r}_i = \overrightarrow{R}_i - \overrightarrow{R}_{i-1}$ $(i = 0, ..., N)$.The letter set representes an ensemble of independent connection vectors .There are two popular static properties by which the special size of a polymer is characterized. For example end-to-end vector $\overrightarrow{R}$ of a given polymer is one of the physical properties that determines how long a given polymer is.

$$\overrightarrow{R} = \sum_{i=0}^{N} \overrightarrow{r} = \overrightarrow{R}_N - \overrightarrow{R}_0 \tag{1.1.1}$$

The averaged over all possible conformations of polymer chain end-to-end vector is zero

$$\left\langle \overrightarrow{R}_N \right\rangle = \sum_{i=0}^{N} \langle \overrightarrow{r}_i \rangle = 0$$

The brackets $\langle\rangle$ denote the ensemble average over all possible conformations of polymer chain.In the case of polymer chain, this means that the probability of the end-to-end vector being R is the same as for being –R,so that the two contributions cancel out. If

however, instead of adding the distance of each step we added the square of the distance, we realise that we will always be adding positive quantities to the total. In this case the sum will be some positive number, which grows larger with every step. This obviously gives a better idea about the distance (squared in this case) that a polymer moves. This can be seen as follow, thus the simplest none zero average is the mean square end-to-end distance

$$\left\langle \overrightarrow{R}^2 \right\rangle = \sum_{i=1}^{N} \sum_{j=1}^{N} \langle \overrightarrow{r_i} . \overrightarrow{r_j} \rangle \tag{1.1.2}$$

Assuming all the bond vectors having the same lenght b and the mean square end-to-end distance is given by

In general case we can express it as in the following equation

$$\left\langle \overrightarrow{R}^2 \right\rangle = \sum_{i=n}^{N} \sum_{m=0}^{N} \langle \overrightarrow{r}_n . \overrightarrow{r}_m \rangle = \sum_{m=0}^{N} \left\langle \overrightarrow{r}_n^2 \right\rangle \delta_{mn} = Nb^2 \tag{1.1.3}$$

Where δ_{mn} is Kronecker delta:

$\delta_{mn} \equiv 1$ for $m = n$

$= 0$ for $m \neq n$.

This shows that the average size of a given ideal polymer chain of N monomers is proportiona to $\sqrt{N}$[4]. For a polymer chain made of N monomers, the mean square of radius of gyration is defined as:

$$\left\langle \overrightarrow{R}_g^2 \right\rangle = \frac{1}{N} \sum_{j=1}^{N} \left\langle (\overrightarrow{r}_i - \overrightarrow{r}_{cm})^2 \right\rangle \tag{1.1.4}$$

where $\overrightarrow{r}_{cm}$ and for large N

$$\left\langle \overrightarrow{R}_g^2 \right\rangle = \left\langle \frac{1}{6} \overrightarrow{R}^2 \right\rangle \tag{1.1.5}$$

Thus , the mean–square radius of gyration of an ideal , linear polymer obeys the same scaling behavior as its mean –square end –to –end vector.

1.1.2 Real polymer chains

In the model of the previous section, we assumed that the orientation of each bond is random and completely independent of the orientation of the previous bond. This means that the polymer is able to fold back on to itself at certain location, which is physically impossible since any two physical bodies can not occupy the same position at the same time. In other words any two monomers in space interact when they come closer to each other. This interaction between segments is called **Excluded Volume Interaction(Effect)**. In reality , two segments cannot occupy the same space at the same time.This interaction between segments is called the excluded volume interaction.The simplest formulation of excluded volume is the self–avoiding random walk, a random walk that cannot repeat its previous path.Because of the self –avoiding nature of this model,the number of possible conformations is significantly reduced. A detailed analysis of real polymer chains was carried out by Flory [8].An important result from Flory's theory for a polymer in good solvent is that it yields a universal power–law dependence of polymer size R on the number of monomers N, i.e

$$\left\langle R^2 \right\rangle \propto N^{2\nu} \tag{1.1.6}$$

where ν

$$\nu = \frac{3}{d+2} \tag{1.1.7}$$

For one dimensional(d) polymer where $\nu = \frac{3}{1+2} = 1, \langle R^2 \rangle \propto N$ and in two dimension,$\nu = \frac{3}{2+2} = \frac{3}{4}$, $\langle R^2 \rangle \propto N^{\frac{3}{2}}$. This shows that equation 1.1.6 is a remarkable result[9]. Moreover, this equation shows that for higher dimension ν found to decrease showing that the end–to–end distance becomes shorter. For instance, for $d = 4$ we see that $\nu = \frac{1}{2}$.

1.2 Polymer translocation

In this part of the thesis we shall discuss the process of translocation of polymer through a small pore and its application in life. The translocation of a polymer through a nano-sized pore occurs as a part of many biological processes and functions, such as DNA(Deoxyribonucleicacid) and RNA(Ribonucleicacid) translocation through nuclear pores, protein transport across membrane holes and virus injection[5-7].The translocation process is also envisioned to have several biotechnological applications, including rapid DNA sequencing, gene therapy and controlled drug delivery. Due to various potential technological applications, such as rapid DNA sequencing, gene therapy and controlled drug delivery [10-11].Polymer translocation has been the subject of a number of experimental, theoretical, and numerical studies[12-14]. In order to overcome a large entropic barrier typical to polymer translocation and to speed up the translocation, an external driving force is needed, such as an electric field, chemical potential difference, or selective adsorption on one side of the membrane. In addition to its biological relevance, the transport dynamics of polymers through nanopores is of fundamental interest in physics and chemistry.Among these mechanisms, less attention has been paid to confinement–driven translocation. In particular its dynamics remains unclear, despite its importance to biological processes including viral ejection, drug delivery, controlled release from a nanopore, etc. Here are interested to investigate the generic behavior of polymer transport into a small hole of cavity from a confined environment.Thus the translocation process includes two essential steps. First, one end of the polymer enters into the cavity directed by Monte Carlo steps and by the action of an extenal field near the cavity. Fig.1.2 Second, the polymer is translocated from one side of the cavity to the other side, driven by an external field. as shown in the Fig.1.3.Hence the existing theories [15-26] provide different predictions for the scaling behavior of the translocation time as a function of polymer length, $\tau \sim N^{1+\nu}$, where ν is the Flory exponent,and N is the polymer size.

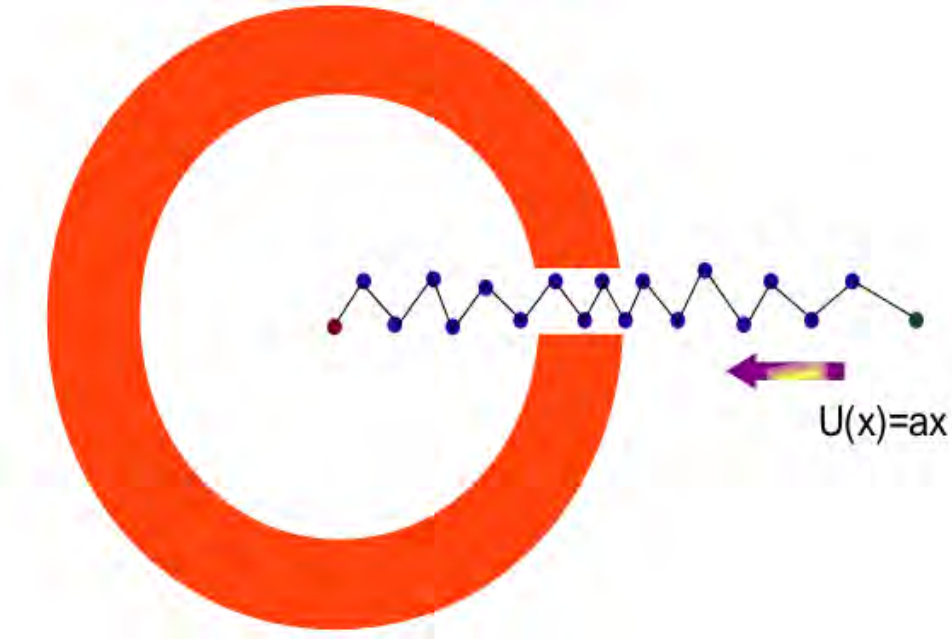

Figure 1.2: Schematic representation of polymer translocation into a cavity hole in a 2D circular compartment driven by an external field during translocation

The three main translocation processes of a polymer chain studied either theoretically or by computer simulation, are:

I .Unbiased translocation,where in the polymer translocates purely due to thermal fluctuations

II . Field-driven translocation, where in the polymer translocation is driven by a potential difference across the pore or an electric field applied, and

III .Pulled translocation, where in the polymer translocation is facilitated by a pulling force at the head of polymer.

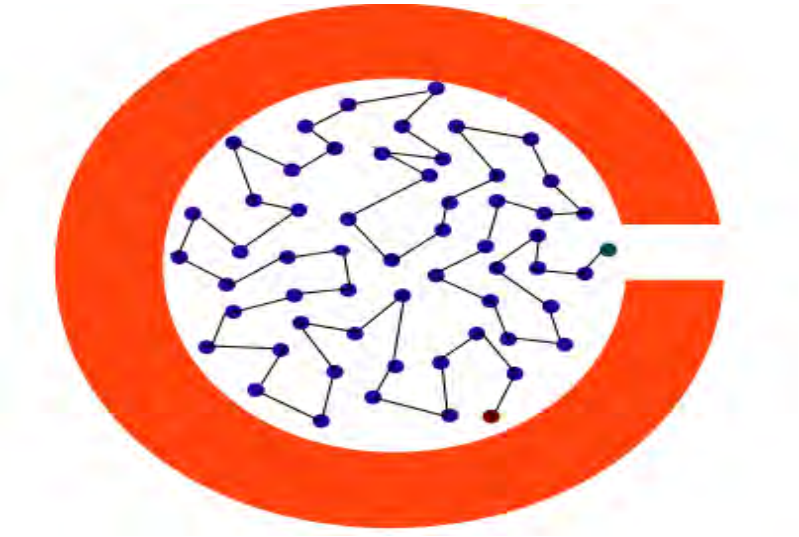

Figure 1.3: Schematic representation of polymer translocation into a cavity hole in a 2D circular compartment driven by an external field after translocation

In this paper to clarify predictions for the scaling behavior we will focus on the biased polymer translocation into a cavity hole.We are studying field driven translocation,so to overcome the entropic barrier we also put the middle monomer tethered mid-way in the cavity hole. We shall discuss this in detail later in chapter two.

Generally, we investigate the field-driven translocation in a 2D lattice model by focusing on only different polymer size.In particular,we shall investigate the effect of varying the chain lenght of the polymer sizes on the escape time.

Chapter 2

Models and Methods

Among the many methods we use the popular techniques to simulate the kind of simulation work is Monte Carlo (MC). As a result one has to make a decision to use one of these according to the problem in hand. If one chooses to use MC, then one has a further choice, namely whether to do the simulation on a lattice. The collective motion of a chain is modeled by the acceptance of an attempted new configuration. Under certain circumstances one can use such an approach not only for static properties but also for the investigation of the dynamics of the system. In such a case the local configurations and the attempted moves are the same as in the case in which one includes the excluded volume interaction between all monomers. In order to fulfill this requirement, it is necessary to structure the algorithm which it will be discussed later.

2.1 Lattice models

2.1.1 Standard lattice algorithm

The self–avoiding walk(SAW) was proposed by Orr and Montroll [27] 50 years ago. The self-avoiding walk (SAW) as a model for a linear polymer in a good solvent. The SAW is defined on a discrete lattice, often on a square . Each monomer occupies one lattice site, the bond length equals the lattice constant. In these algorithms, one chooses a

monomer at random.Since one is dealing with a discretized system, one can use integer arithmetic instead of floating point.This means that determining the distance between two monomers can be done very quickly leading to a very fast update procedure. For large enough memory, as is standard for modern computers, one can store the entire lattice and check the excluded volume constraint simply by checking the occupation of the lattice sites.

2.1.2 Bond fluctuation method

Bond fluctuation model is a lattice model for simulating polymer systems.It was introduced by Carmesin and Kremer in 1988 [28].It is useful for obtaining static and dynamic properties of polymers. According to this model, a trial conformation is generated by moving a randomly selected monomer from its current location to a location one lattice spacing away, along one of the possible directions chosen randomly and with equal probability. During the move we must ensure that bond crossing does not occur and self avoidance condition is satisfied generated by moving a randomly selected monomer. We start with a polymer of required size.A trial conformation, generated by local rule, is accepted or rejected by Metropolis algorithm.

Basic description of the Bond Fluctuation Model (BFM)

On a two dimensional square lattice, every monomer can occupy four lattice sites of a unit cell [31-32]. Each lattice site can at best be part of only a single monomer by virtue of self avoidance condition.We implemented it on a square lattice with lattice constant unity. Let l denotes length of a bond. According to the definition the minimum bond length is $l = 2$. A bond length less than 2 violates self avoidance condition. We restricted to bond length less than 4. This condition ensures that no bond crossing take place .The model is illustrated for a polymer into a cavity of thickness 2 lattice sites in Fig.2.1, with monomer 4 is placing within the hole that is 5 lattice sites wide. Adjacent monomers are connected by a bond, which can only take lengths of [29] are: $2,\sqrt{5},\sqrt{8}$, $3,\sqrt{10}$ and $\sqrt{13}$

Figure (2.1) shows a bond fluctuating lattice polymer with all possible bond lengths. In the present work, we restricted ourselves to four site model[30] on a two dimension square lattice.

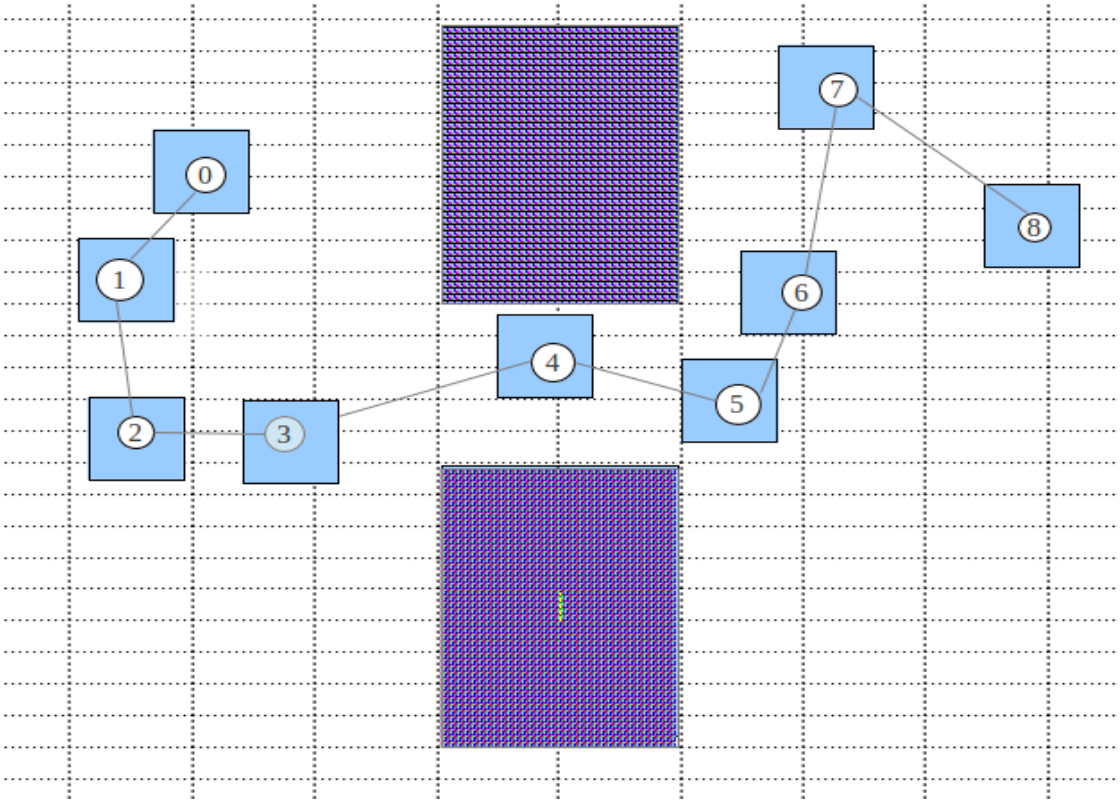

Figure 2.1: A bond fluctuating lattice polymer with all possible bond lengths less than 4 lattice units is depicted.Two monomers, not connected by a bond, but separated by a distance $d \leq \sqrt{13}$.

Algorithm

Implementation of bond fluctuation model proceeds as follow

step1: Start with an initial linear self avoiding conformation of a lattice polymer consisting of N monomers.

step2: Select a monomer randomly and select one of the four lattice directions randomly with equal probability.

step3: Move the selected monomer in the selected direction by one lattice spacing, called this a trial move.

step4: Check if the trial move violates self avoidance condition. If it does, then reject the trial move by placing the monomer in its earlier lattice position and go to step 2.

step5: Check if trial move increases the bond length beyond $\sqrt{13}$. If it does, then reject the trial move by placing the monomer in its earlier lattice position and go to step 2.

If both requirements self avoidance and bond length restrictions are met then take the trial conformation for further processing through Metropolis.

step6: Calculate the energy change ΔE between the new and the old configurations of the system, and if $\Delta E < 0$ the move is accepted, otherwise

step7: Generate a random number r such that $0 < r < 1$

step8: If $r < e^{\frac{-\Delta E}{k_\beta T}}$, accept the move , otherwise

step9: Go to step 2. N elementary moves define one MC time step.

2.2 Simulation procedure

The first thing that we did prepare the lattice because we used lattice model for our simulation.Thus we prepared the square lattice whose size 2000 × 2000. And inside the square lattice we prepared/built/ a circular cavity of internal radius r_1 and external radius r_2 with cavity hole width w and thickness l . In our simulation the wall with the cavity hole (pore) is constructed from a row of immobile monomers arranged in a straight line, with w lattice constant gap or thickness representing the cavity hole.For example a hole of thickness = 2 sites and $W = 5$ lattice sites wide shown in the figure 2.2. The lattice units is small enough to allow only a single monomer to pass through.

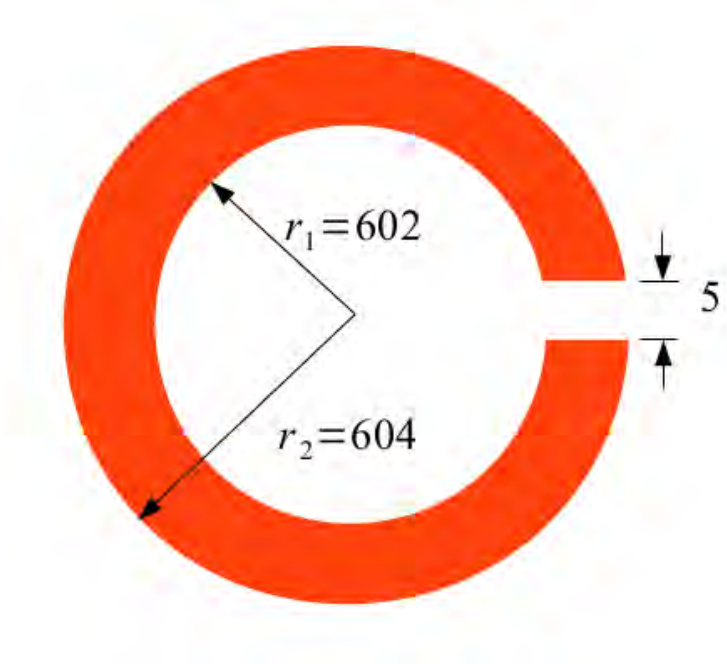

Figure 2.2: Illustration of the confinement cavity employed in this study with thickness 2 sites and 5 lattice sites wide.

Thus in the present work we considered a middle of polymer which is initially placed symmetrically at the center of the hole the reason that we did this all the entropic barrier and the external field so as to make them are equalto zero.Its illustration is given by figure 2.3. To overcome the entropic barrier, i.e, the initial configuration is constructed by fixing the middle monomer $\frac{N}{2}$ in the hole and equilibrating the remaining monomers

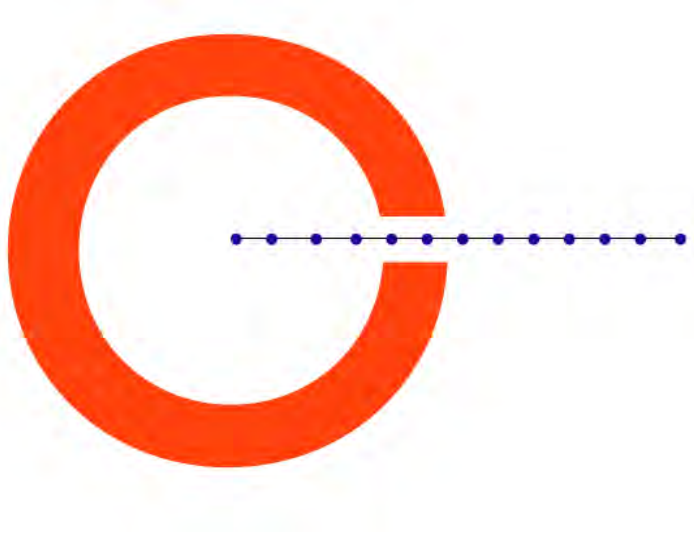

Figure 2.3: Representation of the initial configurations of polymer in the cavity with thickness 2 sites and 5 lattice sites wide

for more than the relaxation or equilibration time $\tau_{equi} \sim N^{1.750}$ in two dimension. After this equilibration is finished, at $t = 0$, the fixed middle monomer is allowed to move freely. as shown in figure 2.4.Thus the simulation ends at a time $t = t' > 0$ when the entire polymer is inside of the circular cavity. This can be done by application of the external field which can be taken as a linear function of the position i.e $U(x) = ax$, where $U(x)$ is the potential x is position and a is constant. and the potential of the polymer due to the external field given by the following equation

$$E_{ext} = \sum_{i=1}^{N-1} U(x_i) \tag{2.2.1}$$

The external potential is applied only outside the cavity :

$$U(x) = \begin{cases} 0 & \text{for } x < x_0 \\ ax & \text{for } x > x_0 \end{cases}$$

where x_0 is the boundary i.e $x_0 = r_1$

It is seen at fig.2.4 where we call this t' is the escape time. This procedure is repeated for a large number of times for each monomer length N. Numerically, τ can be sampled much more efficiently than τ_{tran} , where τ_{tran} is defined as the time that the polymer needs to translocate into a cavity hole by putting the first monomer inside of the circular cavity under a restriction that it never gets back, and the whole translocation process ends when the last monomer is also inside the circular cavity.We will show numerically that $\tau \sim N^{1+\nu}$ in agreement with our simulation result.

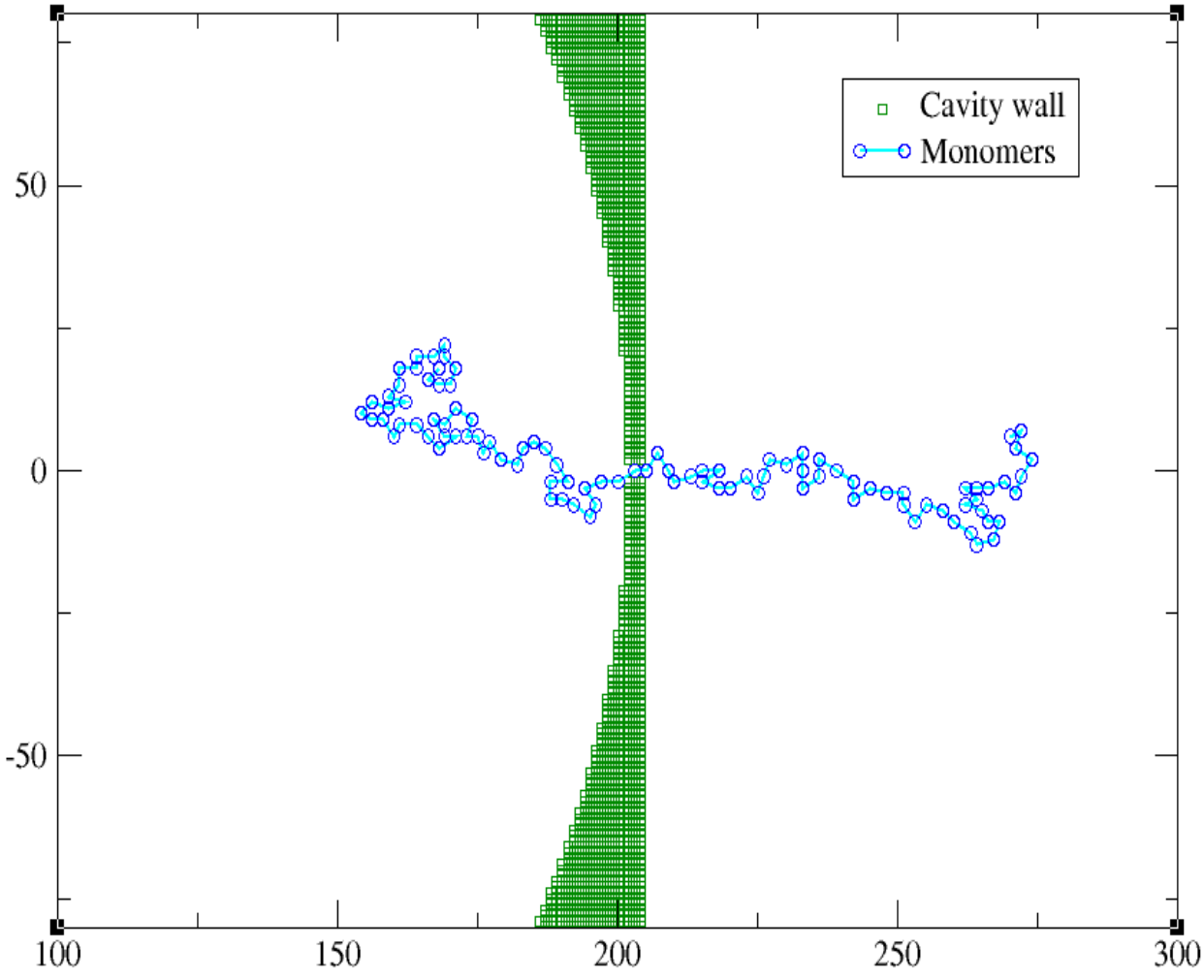

Figure 2.4: Schematic representation of N–monomer polymer in the process of translocation into a circular cavity hole of thickness =2 sites and width w =5 sites with Monte Carlo step of 10^6 and the polymer size , N= 100

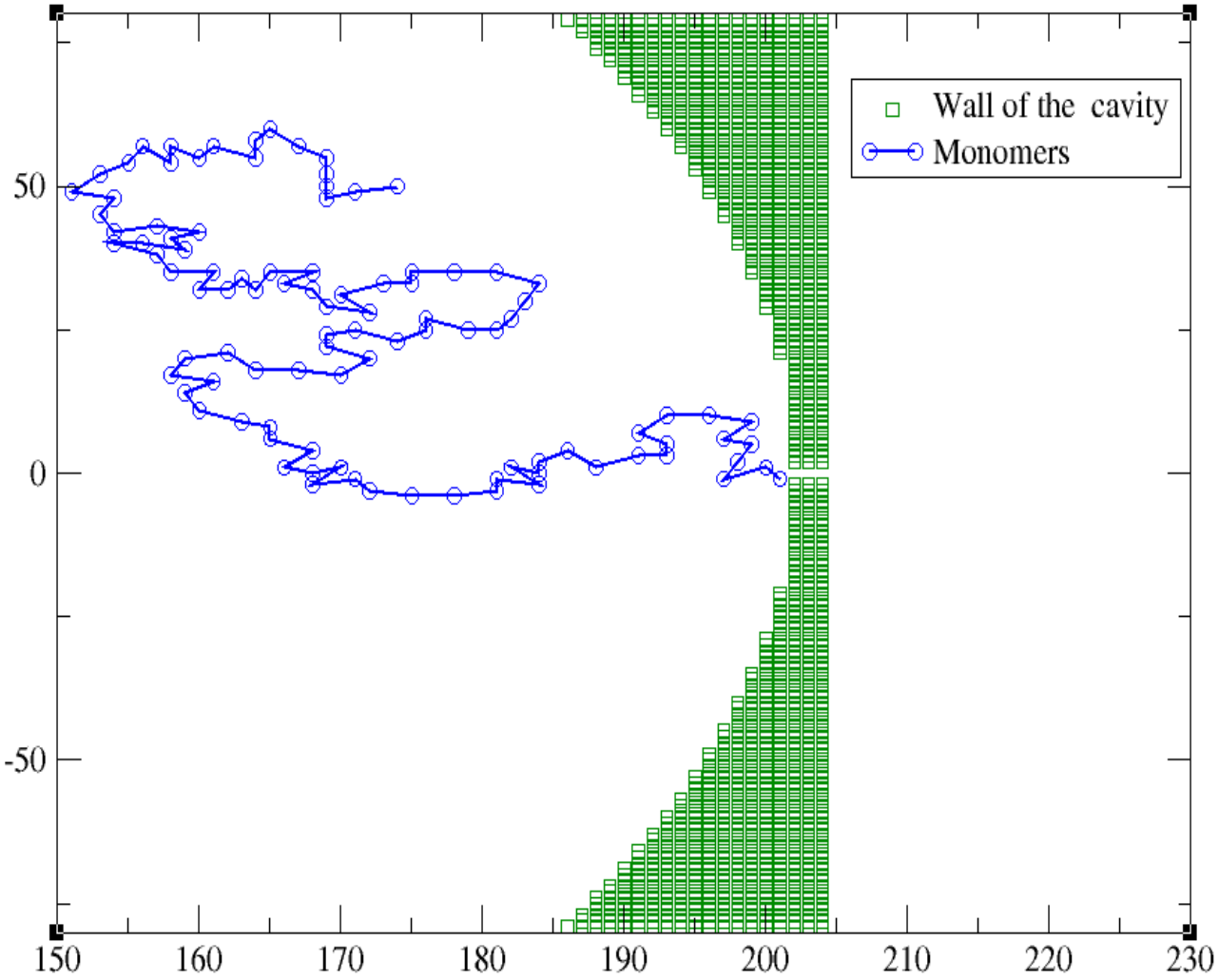

Figure 2.5: Schematic representation of N–monomer polymer after translocation into a circular cavity hole of 2 sites and width w =5 sites with Monte Carlo step of 10^6 and the polymer size , N= 100

The figures are all are taken during our simulation work has been done ,so as to enhance the visibility of the translocation process we used the partial of the circular cavity in both cases. Figure 2.4 shows the freely movement of monomers and starting of the process translocation and figure 2.5 shows that the translocated polymer for single experiment.

Chapter 3

Results and Discussion

3.1 Polymer translocation into a circular cavity

The first thing in this section that we have seen the translocation time or escape time probability distribution function for polymer translocation this helps to find out the most probabile translocation time as a result of this we could be able to examine that the relation shipe between the escape time τ and the polymer chain length N for constant cavity thickness and width. Simply by drawing the graph of escape time versus polymer size and taking logarithmic of their graph and we can compute the slope of the graph that helps to compare our simulation result and the experimental value of Flory exponent in 2D for forced translocation.Since the Flory exponent is the efficience of polymer translocation. However there are so many factors which influences of the translocation or escape time of the polymer translocation ,the driving field stregth,the width of the cavity and the interaction between the cavity wall and the translocated numbers of monomers.

3.1.1 Probability distribution function of translocation time

Additional information about the translocation process can be obtained from the probability distribution function of translocation times $P(\tau)$. This indicated that this distribution deviates from a Gaussian distribution and may be considerably skewed. Consequently,

the average translocation time is not fully representative of the experimental data. We sampled $P(\tau)$ for different polymer chain lengths of N = 20,50,80 120 and 200 monomers, comparable to the chain length employed in the experimental determination of $P(\tau)$. For escape from a circular cavity As shown in Fig. 3.1, for strong confinement the distribution is narrow and nearly Gaussian. However,at weaker confinement $P(\tau)$ broadens and the skewness becomes clearly visible. Following the experimental analysis [33] we therefore fit the data to an empirical expression of the form $\tau^{a_1} exp(–a_2\tau)$. Just as in the experiments,the exponential term provides a good description of the long–time tail. Based on this we studied the passage (translocation) of a self–avoiding polymer into a circular cavity in two dimensions. To do this we tried to see the distribution of the escape times of a polymer as function different chain length polymer sizes.We numerically measure the probability distribution $P_N(\tau)$ of the escape time τ. Figure 3.1 shows the probability distribution function for $P_N(\tau)$ of the polymer which have 5 different sizes i.e the polymer size N= 20, 50, 80, 120 and 200.

3.1.2 Translocation time as function of radius of cavity (r)

In this part of the work we have presented the simulation result of the translocation time as function of radius of the cavity r, from the result that we found when the radius of the cavity increases then the escape time remains constant and for small radius of the cavity escape time increases as result of the more squeezeness of the polymer so as to compactable to the narrow cavity i.e the more squeezeness needs more escape time into the cavity hole as shown in the figure 3.2 below.

3.1.3 Translocation time as function of the chain length (N)

In this section of thesis we presented the results for the escape time τ for a lattice model of polymers. For the same model, we also studied the translocation time τ_{tran} by using the restriction that the first polymer cannot back out of the circular cavity. We used

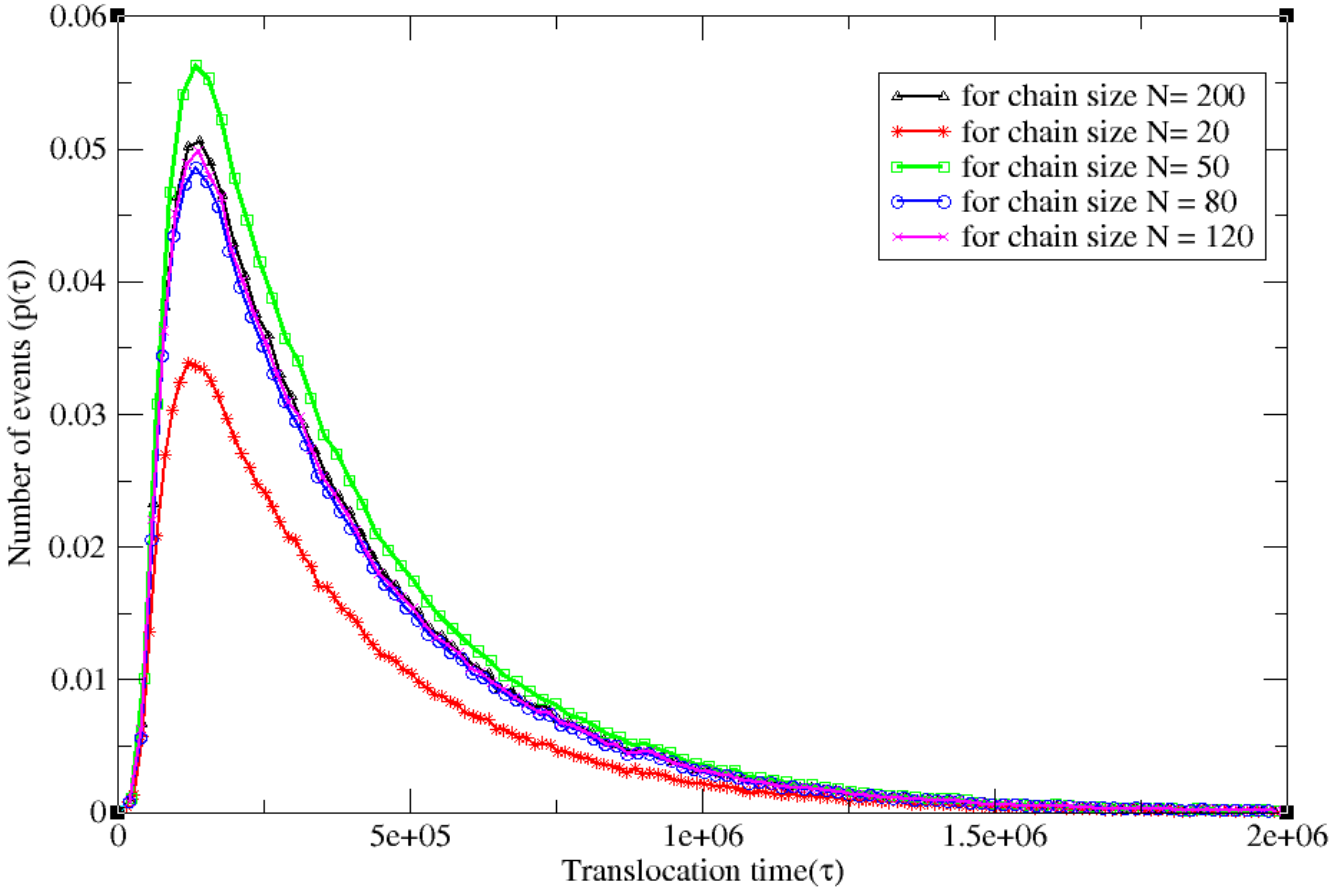

Figure 3.1: Probability distribution $P(\tau)$ of translocation times τ , for a polymer chain lengths of N = 20,50,80,120 and 200 monomers confined into a circular cavity hole. The translocation times are expressed in units of 10^6 Monte Carlo sweeps. The narrow distribution corresponds to a strongly confined chain

the same pore/hole/ size for both cases (thickness of $L = 2$ and width of $w = 5$ lattice units). Numerical studies were done for a number of different chain lengths N,with several thousand runs for each case. To this end as discussed in section our simulation setup, the middle of monomer is placed at the center of the pore; so that the polymer can escape from the pore of circular cavity in a time defined as escape time τ.

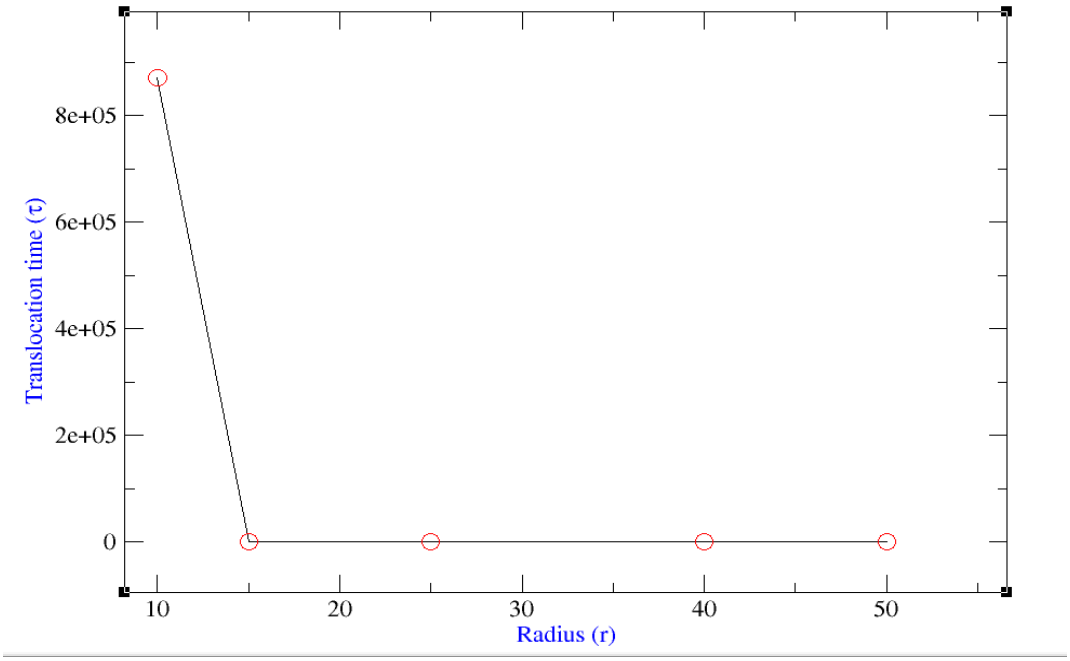

Figure 3.2: A polymer length 50 monomers units

We simulated the escape time of for polymer chains for the scale of τ and took the escape time value which happened mostly. Interestingly the Flory exponent ν has been seen to influence the scaling of the escape time.

The log-log plot of of the most probabile escape time versus the different polymer chain sizes is shown in the figure 3.3 which shows that $\tau \sim N^{\alpha}$ where we find α to $\alpha = 1.75 \pm 0.01$.We found that $\tau_{tran} \sim N^{1.79 \pm 0.01}$ and the result is very close to the expected value of $1 + \nu = 1.75$ in agreement with $1 + \nu$ with slight change.Thus the scaling of $\tau \sim N^{1+\nu}$ implies that τ scales of the polymer chain.

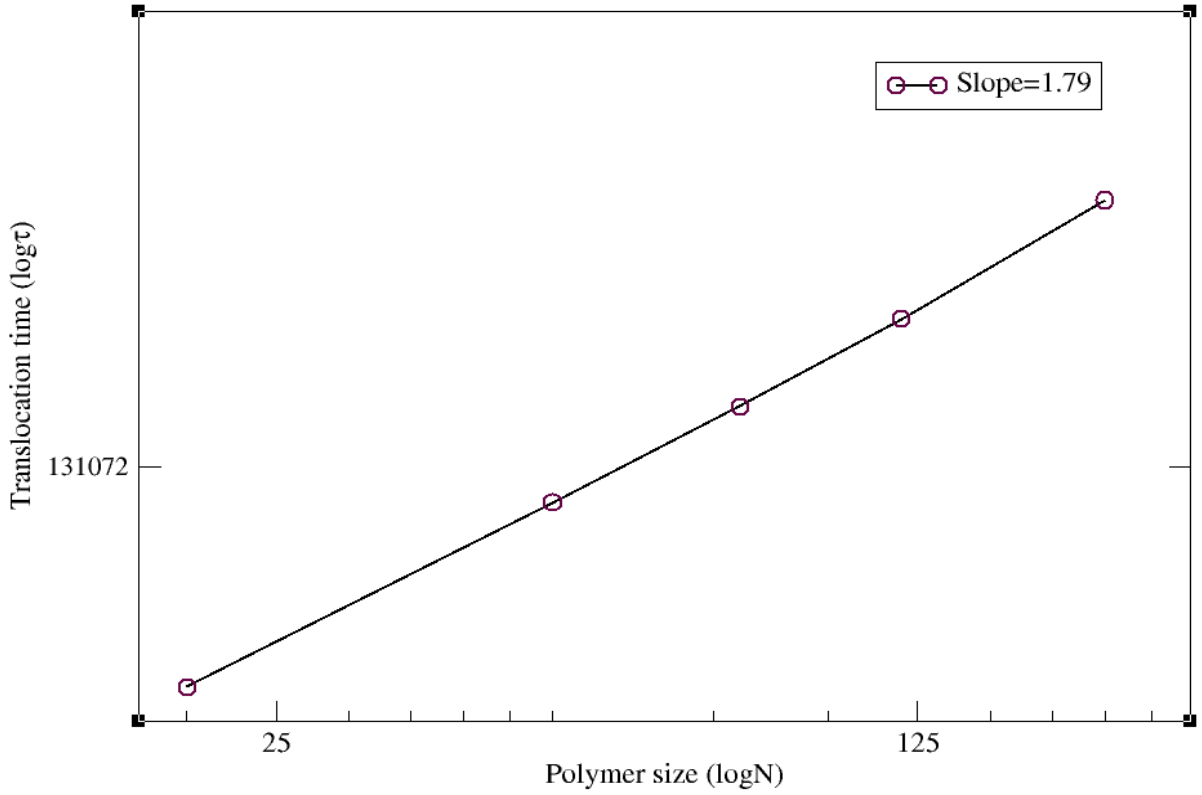

Figure 3.3: Logarithmic plot of the translocation time τ as function of the different chain lengths N of a linear polymer in 2D from a circular cavity hole .The translocation times are expressed in units of 10^6 Monte Carlo sweeps.

Chapter 4

Conclusion

In this paper, we presented the Monte Carlo simulations of simple lattice models of a polymer chains.The chains were put into the Monte Carlo cavity with walls impenetrable to the polymer chains. We have investigated the problem of polymer translocation into circular cavity hole under an external field based on the 2D fluctuating bond model with single–segment Monte Carlo moves.Here among the many influences of on polymer translocation we have examined the influence of of polymer chain length on forced polymer translocation into cavity hole.It was shown that the translocation time of a polymer chain depended on the chain length. The time of translocation depended on the chain length roughly as $N^{1.78}$ which was very close to the other theoretical findings $N^{1.75}$. As our main result , we have found that a crossover scaling for the translocation time with chain length where the escape time τ with the polymer length N satisfies $\tau \sim N^{1+\nu}$. $\tau \sim N$ is obseved .With increasing N there is a high density of segments near the cavity hole due to the slow relaxation of chain which slows down the translocation process. Therefore the translocation time of the translocation phenomenon under forced translocation into a circular cavity is directly proportionla with the length of polymer's chain.

Biblography

[1] A. Yu. Grosberg and A. R. Khokhlov, Giant Molecules, Academic Press, San Diego, 1997

[2] Michael Rubinstein . Aalph H. Colby. Polymer Physics. Oxford University Press, 2003.

[3] Masao Doi. Introduction to Polymer physics. Clarendon Press, Oxford, 1996.

[4] Yaneer Bar-Yam. Dyanmics of Complex system. Westview Press, USA, 1997

[5] B. Alberts et al., Molecular Biology of the Cell, 5th Ed. (Garland, New York) 2008

[6] S. W. P. Turner, M. Calodi, and H. G. Craighead, Phys. Rev. Lett. 88, 128103(2002).

[7] Kehong Zhang and Kaifu Luo, J. Chem. Phys. 136, 185103 (2012)

[8] Michael Rubinstein.Aalph H. Colby. Polymer Physics. Oxford University Press,2003

[9] Paul C.';Coleman ,Michael M. (1997).Fundamental of polymer science: an introduction text.Lancater,Pa.: Technomic Pub.Co.P.1. ISBN 1-56676-559-5

[10] J. Han, S. W. Turner, and H. G. Craighead, Phys. Rev. Lett. 83, 1688 (1999).

[11] D.-C. Chang, Guide to Electroporation and Electrofusion (Academic, New York,1992)

[12] A. J. Storm, C. Storm, J. Chen, H. Zandbergen, J.-F. Joanny, and C. Dekker, Nano Lett., 5, 1193 (2005).

[13] J. Chuang, Y. Kantor, and M. Kardar, Phys. Rev. E 65, 011802 (2001).

[14] Y. Kantor, and M. Kardar, Phys. Rev. E 69, 021806 (2004).

[15] W. Sung and P. J. Park, Phys. Rev. Lett. 77, 783 (1996).

[16] M. Muthukumar, J. Chem. Phys. 111, 10371 (1999).

[17] A. Milchev, K. Binder, and A. Bhattacharya, J. Chem. Phys. 121, 6042 (2004).

[18] K. F. Luo, T. Ala-Nissila, and S. C. Ying, J. Chem. Phys. 124, 034714 (2006).

[19] S.-S. Chern, A. E. Cardenas, and R. D. Coalson, J. Chem. Phys. 115, 7772 (2001).

[20] H. C. Loebl, R. Randel, S. P. Goodwin, and C. C. Matthai, Phys. Rev. E 67,041913 (2003).

[21] R. Randel, H. C. Loebl, and C. C. Matthai, Macromol. Theory Simul. 13, 387(2004).

[22] Y. Lansac, P. K. Maiti, and M. A. Glaser, Polymer 45, 3099 (2004).

[23] C. Y. Kong and M. Muthukumar, Electrophoresis 23, 2697 (2002).

[24] Z. Farkas, I. Derenyi, and T. Vicsek, J. Phys.: Condens. Matter 15, S1767 (2003).

[25] P. Tian and G. D. Smith, J. Chem. Phys. 119, 11475 (2003).

[26] R. Zandi, D. Reguera, J. Rudnick, and W. M. Gelbart, Proc. Natl. Acad. Sci.U.S.A. 100, 8649 (2003).

[27] W. J. C. Orr, Trans. Faraday Soc. 43, 12 (1947); E. W. Montroll, Markoff Chains and Excluded Volume Effects in Polymer Chains, J. Chem. Phys. 18, 734 (1950)

[28] I. Carmesin and K. Kremer, Macromolecules 21, 2819 (1988).

[29] P. J. Flory, Statistical Mechanics of chain molecules, Interscience, New York (1969).

[30] M. Rubinstein and R. H. Colby, Polymer Physics, Oxford University Press, New York (2003).

[31] L. Carmesin and K. Kremer, The bond fluctuation method: a new effective algorithm for the dynamics of polymers in all spatial dimensions, Macromolecules 21, 2819 (1988).

[32] K. Binder, Monte Carlo and Molecular Dynamics Simulations in Polymer Science, Oxford University Press (1995).

[33] A. Meller, L. Nivon, and D. Branton, Phys. Rev. Lett.86, 3435 (2001).

Declaration

This thesis is my original work, has not been presented for a degree in any other University and that all the sources of material used for the thesis have been dully acknowledged.

Name: Fikre Jida

Signature:– – – – – – – – – – – –

Place and time of submission: Addis Ababa University, June 2013

This thesis has been submitted for examination with my approval as University advisor.

Name: Dr.Tatek Yergou

Signature:– – – – – – – – – ––