Dynamics Of XY Model And Analogy With Non-Newtonian Fluid

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Certificate of Examination

This is to certify that the dissertation titled **"Dynamics Of XY Model And Analogy With Non-Newtonian Fluid"** submitted by **Deepu S** (Reg. No. MS15069) for the partial fulfillment of BS-MS dual degree program of the Institute, has been examined by the thesis committee duly appointed by the Institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

Dr. Rajeev Kapri Dr. Abhishek Chaudhuri Dr. Sanjeev Kumar

(Supervisor)

Dated: June 12, 2020

Declaration

The work presented in this dissertation has been carried out by me under the guidance of Dr. Sanjeev Kumar at the Indian Institute of Science Education and Research Mohali.

This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgement of collaborative research and discussions. This thesis is a bonafide record of original work done by me and all sources listed within have been detailed in the bibliography.

Deepu S

(Candidate)

Dated: June 12, 2020

In my capacity as the supervisor of the candidate's project work, I certify that the above statements by the candidate are true to the best of my knowledge.

Dr. Sanjeev Kumar

(Thesis Supervisor).

Acknowledgement

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Deepu S

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Abstract

Classical one-dimensional XY model has been proven to imitate some characteristics of non-Newtonian fluids. In this work we study the dynamics of rotors present in an XY system when administered between counter rotating boundaries. As shown in a research paper [Evans 15], we applied Langevin dynamics to 1D XY system to replicate the results which proposed its analogous nature with non-Newtonian fluid. Different distinct types of flow regimes were observed under different combination of system parameters. Then the one chain system was modified to two chain system with the chains aligned parallel and perpendicular to each other. They were also evolved under different combinations of system parameters. We attempted to understand how such a change would affect and alter the dynamics of the system.

Chapter 1

Introduction

Condensed matter physics is the field of physics that deals with the study of microscopic and macroscopic properties of matter using physical laws. Some of the very interesting properties which are studied in this field of physics include ferromagnetic and antiferromagnetic properties of materials studied based on the orientation of spins, superconductivity of certain materials at low temperature, Bose-Einstein condensate and so on. Our deeper understanding of such intricate phenomenon have definitely paved way for the advancement of science and technology further. Applications of condensed matter physics range from identifying the most suitable material fit to make tools used in daily life, like telecommunication devices such as cellphones and other multimedia devices, to superconducting magnets that are used in NMR tomography in medical diagnostics. To understand the plethora of properties exhibited by diverse systems, we use different theoretical models which suit each system uniquely. Classical XY Model [Kosterlitz 73] is one such paradigm among many others in the field of condensed matter physics. Even though it is commonly used to study simple magnetic systems and its properties that first inspired it, Classical XY model's application extends far beyond these systems.

1.1 XY Model

An XY model consists of rotors or spins, s at each lattice site j of the system which is free to rotate in two dimensions, that is, in a plane. Hence each spin has one continuous degree of freedom, θ_j, of the two-component spin vector $s_j = (\cos\,\theta_j\ ,\ \sin\,\theta_j)$. These angles, can acquire any values ranging from zero to 2π, that is

$$0 \leq \theta_j \leq 2\pi$$

To study any system and various phenomenon exhibited by it, we need to understand how the energy dynamics of the system works and generally for an XY system energy corresponding to the configuration of the system is given by the Hamiltoninan,

$$H = \sum_{i,j} J_{ij} s_i . s_j$$

where J_{ij} represent the strength of coupling between ay rotors. There are some systems in which a spin interacts only with its immediate neighbours, for such systems J_{ij} will be zero except for the cases where i and j are neighbours.

The probability of each state or configuration occurring given by,

$$Probability,\ P = \frac{1}{Z}\, exp\,(\frac{-E}{K_B T})$$

Where Z is the partition function of the system, K_B is the Boltzmann's Constant, T is the temperature of the system and E is the energy of the system for that particular configuration.

1.2 Langevin Equation

Langevin Equation is a stochastic differential equation originally developed to describe Brownian motion, which is the random jittery motion exhibited by small particles suspended in a fluid. Brownian motion was first experimentally observed by a Scottish botanist Robert Brown [Brown 28] when he was observing the motion of pollen grains suspended in water using a simple microscope. However a theoretical explanation was only provided by Einstein [Einstein 56] way after its discovery. Brownian motion was later extended to some collective properties of macroscopic systems instead of just fluctuating particles. The Langevin Equation contains frictional and random noise terms apart from the classical force terms. Since we are dealing with multiple rotors rotating simultaneously in a chain, this equation is also applicable in the XY system.

The Newton's equation of motion governing the motion of a Brownian particle in one dimension is given by,

$$m\frac{dv}{dt} = F_{tot}(t)$$

where m is the mass of the Brownian particle and $F_{tot}(t)$ is the total force acting on the particle. Since the source of the force acting on the particle is mainly the viscous force exerted by the fluid medium on the particle, the above equation can be re-written as,

$$m\frac{dv}{dt} = -\zeta v$$

where ζ is the friction constant, v is the velocity of the particle. On solving the above differential equation we get

$$v(t) \;=\; v(0)e^{\frac{-\zeta t}{m}}$$

Hence based on this equation, velocity of the particle should decay to zero for infinitely long time duration. But this is in contradiction to the Maxwell-Boltzmann distribution law which states that the mean squared velocity of a particle in thermal equilibrium should be $\frac{K_B T}{m}$. Therefor the assumption that only the frictional force of the medium is involved has to be corrected. At each instant the Brownian particle is colliding with a large number of particles in the fluid medium. The number of collisions and the force exerted by these particles varies at each instant. So we bring in this random colliding force into the picture by adding one more term to the differential equation, that is,

$$m\frac{dv}{dt} = -\zeta v + \delta F(t)$$

$\delta F(t)$ is the Gaussian white noise term acting on the rotor at time instant t. Properties of the white noise term are:

$$\langle \delta F(t) \rangle = 0$$

$$\langle \delta F(t) \delta F(t') \rangle = 2B\delta(t - t')$$

The first equations states that the time average of the noise term is always zero. And the second equation states that there is absolutely no correlation between between the random noise terms at two different time instances. This is known as the auto-correlation function of the white noise. The variable B indicates the intensity of the fluctuating force. In the presence of external force the Langevin Equation is defined as

$$m\frac{dv}{dt} = F - \zeta v + \delta F(t)$$

where F is the external force acting on the system.

1.3 Non-Newtonian Fluid

Non-Newtonian fluids are those fluids which do not obey Newton's Law of viscosity, which states that there is a linear relation between stress and shear rate. So for Newtonian fluids, the proportionality constant η, known as *Viscosity*, will be constant throughout the fluid for a given temperature, no matter how fast the fluid is flowing through a channel.

Unlike Newtonian fluids, in non-Newtonian fluids the relation between stress and shear rate is not linear and therefore one cannot observe a constant viscosity through out the fluid. They show macroscopic regions with different shear rate existing simultaneously.

According to a research paper published by R.M.L Evans *et. al* [Evans 15], one-dimensional XY model with conserved angular momentum and counter rotating boundaries is analogous to non-Newtonian fluids and exhibits non-Newtonian fluid flow characteristics. Based on the trend in which the shear rate is distributed along the fluid, flow regimes can be classified into the following regimes.

1.3.1 Uniform Flow Regime

This type of flow regime shows constant shear rate throughout the fluid. It exhibits characteristics of a Newtonian fluid with linear relation between stress and shear rate. Therefore the global shear rate is same as the local shear rate at any layers of the fluid. This characteristic kind of fluid flow is shown by almost all fluids. If fluids don't exhibit this kind of flow characteristic at normal conditions, we can observe it in the same fluid at a higher temperature.

1.3.2 Shear Banding Regime -SBR

This type of flow regime shows different sections of layers of the fluid having different shear rates. These specific regions or layers having different shear rates are fairly distinguishable and are identified as different *Bands*, hence the name Shear Banding. Some polymers [Kunita 12], colloids [Besseling 10] and surfactant phases [Schmitt 94] exhibit this particular flow regime characteristics.

1.3.3 Solid- Fluid Coexistence Regime

This type of flow regime shows different separated regions or layers with features of solid interconnected by layers showing characteristics of fluids. Solid region is marked by layers of fluid with constant velocities and hence zero shear rate. And liquid region is marked by layers of fluid having uniform shear rates between the solid regions. This particular flow characteristic is shown by some foams [Debregeas 01] and colloids [**?**]. Some fluids even show both solid-fluid coexistence characteristics as well as slip planes.

1.3.4 Slip-Plane Regime

This type of flow regime is characterised by the presence of multiple sections of fluid with solid nature, marked by the presence of layers of fluid with constant velocities. There are no layers of fluid in between these sections with any other distinct velocities. Hence all of the shear flux is concentrated between non-connected solid sections known as *Slip Planes*. This particular fluid flow is observed in some surfactant cubic phases [Jones 95] and polymer melts [Tapadia 03].

Chapter 2

One Chain System - 1D XY Model

One dimensional XY Model is a simple XY model consisting of only a single chain of rotors. The plane of rotation of the rotors is perpendicular to the spatial location of the rotors on the axis of the chain.

2.1 Model Description

In this particular one chain XY system which we consider, the rotors or spins couple only to their immediate neighbours. The intra-chain coupling constant J_{ij} is one here and the system is $Spin\,1$ system, that is, $s_j = 1$ at all lattice points j. Consequently, the Hamiltonian of the system is given by,

$$H = \sum_{j=1}^{N} [-s_j.s_{j-1} + \frac{1}{2}\dot{\theta}_j^2]$$

where the first term in the Hamiltonian represent potential energy due to the spin coupling between two neighbouring spins. This energy is dependent on the

relative orientation between those two specific rotors. And the second term in the Hamiltonian represent the rotational kinetic energy of a rotor, which is dependent only on the rotational velocity of that rotor.

Since we are only interested in the non-equilibrium behaviour of the system, we add two counter rotating rotors, driving rotors, one on either side of the chain. These rotors are made to rotate relentlessly at a constant velocity in time and therefore continuously supply energy to the system.

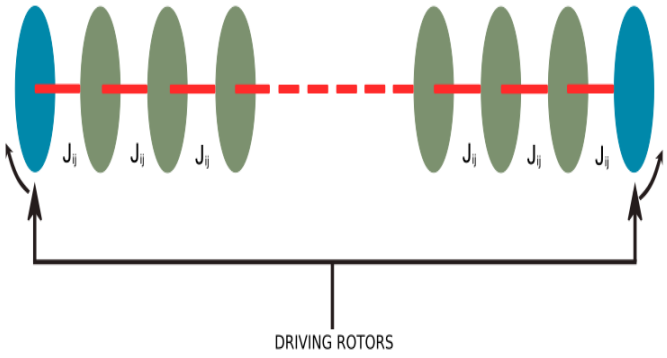


Figure 2.1: Schematic representation of 1D XY system. The blue ellipses at both ends represent counter rotating driving rotors.J_{ij} is the intra-chain coupling constant.

2.2 1D XY Model and Non-Newtonian Phenomenology

Even though 1D XY model exhibits trivial equilibrium phase behaviour, away from equilibrium the system seem to imitate the characteristics of non-Newtonian fluids. It maybe challenging for someone at first to find a connection between a condensed matter system like XY model and a classical physical system like Non-Newtonian fluid. The analogy between one dimensional XY system and fluid system can be understood by visualizing that the rotation of spins in 1D XY system is similar to the rotation of different layers of fluid in a parallel-plate rheometer [Unterberger 14] [Tempel 96]. The rotational velocity difference of the rotors can be used to represent shear rates.

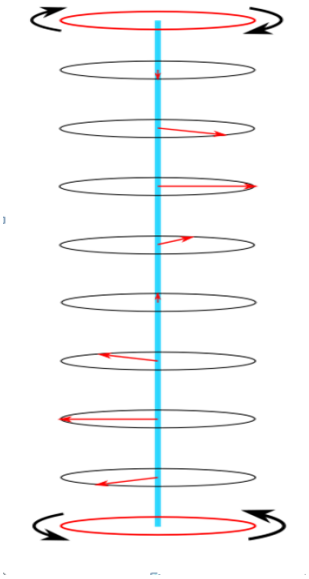


Figure 2.2: Diagrammatic representation of 1D XY system. The two red ellipses, which is the trajectory of driving rotors, can be considered as the rotating parallel plates of a rheometer and the black ellipses,trajectory of other spins, can be considered as different layers of fluid in between these plates. The red arrows represent the rotating spins.

2.3 Model Simulation

Even though model's dynamics may not affect the phase behaviour of the system at equilibrium, we need specific equations of motion to determine the dynamics of the system in non-equilibrium. Here we apply Langevin dynamics to develop and study the system. The forces involved obey Newton's Laws of Motion and hence conserve angular momentum of the rotating spins, which only have angular degrees of freedom and no radial motion. The frictional and stochastic part of the Langevin equation only act between nearest neighbours. Using Hamilton's equation to find generalized momenta τ_j and incorporating the the frictional and stochastic parts of the Langevin equation, we get the dynamical equations for the system. The equations are

$$\ddot{\theta}_j \;=\; \tau_j - \tau_{j-1},$$

$$\tau_j \;=\; \sin\Delta\theta_j + \mu\Delta\dot{\theta}_j + \eta_j(t)$$

Here, τ_j is the torque applied by rotor j+1 on rotor j. $\Delta\theta_j$ is the relative angular difference between rotors at lattice points $j+1$ and j, that is, $\Delta\theta_j \;=\; \theta_{j+1} - \theta j$. μ is the coefficient of friction and $\eta_j(t)$ is the δ-correlated Gaussian function with mean zero and,

$$\langle\eta_j(t)\eta_j(t')\rangle \;=\; 2\mu T\delta(t-t')\delta_{ij}$$

The simulations were done with $k_B \equiv 1$ at a temperature, T, and μ was same for all rotors, including the driving rotors. Dissipative Particle Dynamics (DPD) algorithm [Groot 97] was used to evolve the system. Finite size effect was eliminated by setting the total number of rotors to be $512(N)$. An overall global shear rate was given to the system by giving specific velocity difference$(N\dot{\gamma})$ between the counter rotating driving rotors. So the system as a whole experience a mean shear rate, angular difference per rotor, $\dot{\gamma}$.

2.4 Results

The combination of system variables, namely temperature T, co-efficient of friction μ and mean shear rate γ determined the behaviour of the system. On evolving the model at different system parameters for asymptotically late times $t \geq 4500$ and averaging of rotors over 500 units of time, four distinct type of flow regimes were observed. they are,

- Uniform Flow Regime at $(T, \mu, \dot{\gamma}) = (0.02,50,0.009960)$
- Shear Banding Regime at $(T, \mu, \dot{\gamma}) = (0.02,10,0.007813)$
- Solid-Fluid Coexistence Regime at $(T, \mu, \dot{\gamma}) = (0.001,1,0.0078125)$
- Slip Planes Regime at $(T, \mu, \dot{\gamma}) = (0.001,0.5,0.0058938)$

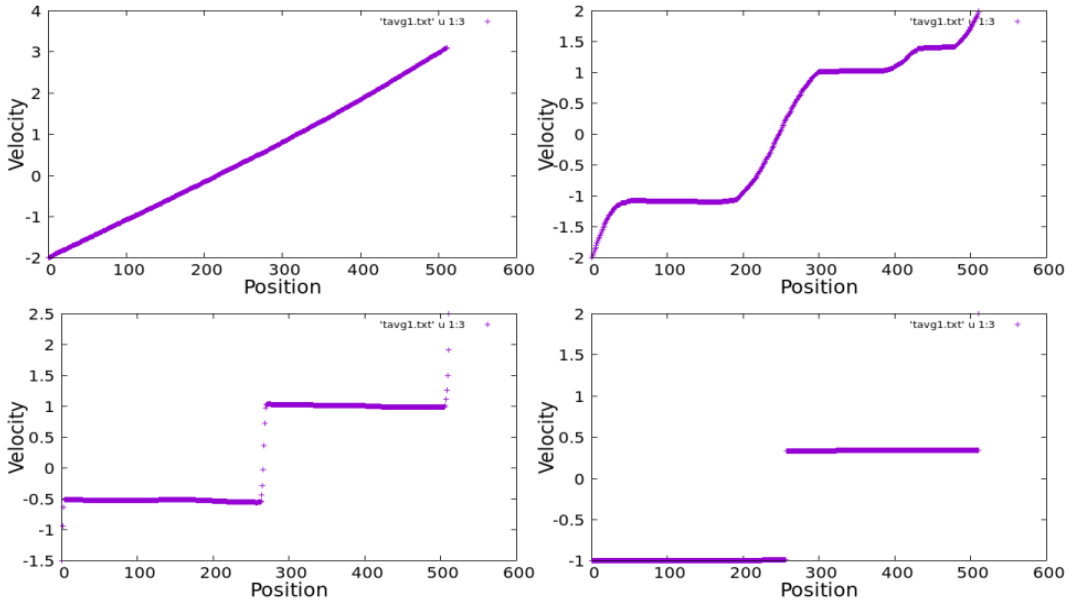


Figure 2.3: Angular velocity versus position in a chain of 512 rotors showing four different flow regimes. (a) Unform; (b) Shear Banding; (c) Solid-Fluid Coexistance; (d) Slip Planes

Chapter 3

Two Chain Systems - Quasi 1D Model

Quasi one dimensional XY Model is another simple XY model consisting of two single chain of rotors where it is not essentially a two dimensional system. The plane of rotation of each rotor will be perpendicular to their spatial location on the axis of the chain they belong to.

3.1 Parallel Two Chain System

3.1.1 Model Description

In this particular two chain XY system which we consider, the rotors or spins couple only to their immediate neighbours as in 1 chain system. Since there are two chains, say *chain a* and *chain b*, each rotor will have three interaction terms, two from the neighbours present on it's either side on the same chain and one from the rotor present at the corresponding lattice point on the parallel chain. The intra-chain coupling constant J_{ij} is one here for both the chains and the

system is *Spin* 1 system, as before. The strength or intensity of the interaction of rotors between the two chains is determined by the inter-chain cAoupling constant, α. Consequently, the Hamiltonian of the rotors present in *chain a* is given by,

$$H = \sum_{j=1}^{N} -s_j^a.s_{j-1}^a - \alpha s_j^a.s_j^b + \frac{1}{2}(\dot{\theta}_j^a)^2$$

Similarly the Hamiltonian of rotors present in *chain b* is given by,

$$H = \sum_{j=1}^{N} -s_j^b.s_{j-1}^b - \alpha s_j^a.s_j^b + \frac{1}{2}(\dot{\theta}_j^b)^2$$

where the superscripts a and b represent the chain in which the rotor belongs to. The first two terms in the Hamiltonian represent potential energy due to the spin coupling, first term comes from the coupling between spins on the same chain and the second term comes from coupling between spins on different chain. These potential energy terms are dependent on the relative orientation between two specific rotors. And the third term in the Hamiltonian represent the rotational kinetic energy of a rotor, which is dependent only on the rotational of that rotor.

Like before, to study the non-equilibrium behaviour of the system, we drive the system out of equilibrium by adding two counter rotating driving rotors, one on either side of both the chains. These rotors rotate continuously at a constant velocity in time.

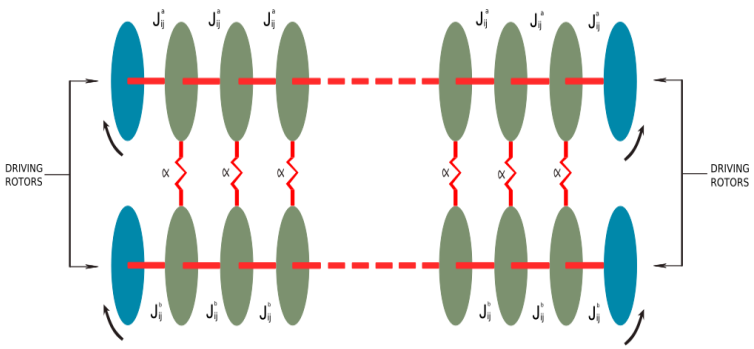


Figure 3.1: Schematic representation of parallel two chain XY system. The blue ellipses at both ends represent counter rotating driving rotors. α is the inter-chain coupling constant and J_{ij} is the intra-chain coupling constant of the respective chains

3.1.2 Model Simulation

Here also we apply Langevin dynamics to develop and study the system. The nature of forces and motion of rotors are same as those in the one chain system. The added inter-chain interaction also obey Langevin dynamics. The modified dynamical equations for the system are as follows.

for rotors in *chain a*,

$$\ddot{\theta}_j^a = \tau_j^a - \tau_{j-1}^a - \tau_j^b,$$

for rotors in *chain b*,

$$\ddot{\theta}_j^b = \tau_j^b - \tau_{j-1}^b + \tau_j^a,$$

In both the equations the first two terms represent torque exerted on a rotor by it's neighbouring rotors on the same chain. The expression for these torques is same for both chains.

$$\tau_j = \sin\Delta\theta_j + \mu\Delta\dot{\theta}_j + \eta_j(t)$$

Here, τ_j is the torque applied by rotor $j+1$ on rotor j present on the same chain and $\Delta\theta_j$ is the relative angular difference between rotors at lattice points $j+1$ and j on the same chain, that is, $\Delta\theta_j = \theta_{j+1} - \theta j$.

The third term in both acceleration function is due to inter-chain interaction. For a rotor in *chain a* this will be due to the corresponding rotor at the same lattice point j on *chain b*. Similarly for a rotor in *chain b* this will be due to the corresponding rotor at the same lattice point on *chain a*. The intensity or strength of this interaction is scaled by the inter-chain coupling constant α. The magnitude of effect of this torque will be same for rotors on both the chain, but its direction will be opposite as shown in the acceleration functions.
Expression for this torque is,

$$\tau_j = \sin\Delta\theta_j + \mu\Delta\dot{\theta}_j + \eta_j(t)$$

Here, τ_j is the torque experiences by rotor at lattice point j on *chain a* by rotor at the same lattice point j on *chain b* or vice-versa. $\Delta\theta_j$ is the relative angular difference between rotors at lattice point j on both chains, that is, $\Delta\theta_j = \theta_j^a - \theta j^b$.

μ is the coefficient of friction and $\eta_j(t)$ is the usual δ-correlated Gaussian function with mean zero.

The simulations were done with $k_B \equiv 1$ at a temperature T, and μ was same for all rotors, including the driving rotors. Like before, Dissipative Particle Dynamics (DPD) algorithm was used to evolve the system. Number of rotors on both chains were set to 512 to eliminate finite size effect. The inter-chain coupling constant, α was constant for all inter-chain interactions. Apart from the combination of usual three variables, T, μ and $\dot{\gamma}$, now α also determined the behaviour of the system. So the system was studied at different values of α also.

3.1.3 Results

The model was evolved at different system parameters corresponding to different flow regimes. They were also simulated for different values of inter-chian coupling consatnt, α. The system was evolved for asymptotically late times $t \geq 4500$ and the of rotors were averaged over 500 units of time. The results obtained are shown below. In the plots violoet markers indicate the of rotors in *chain a* and green markers indicate the of rototrs in *chain b*.

- Uniform flow regime environment at $(T, \mu, \dot{\gamma}) = (0.02{,}50{,}0.009960)$

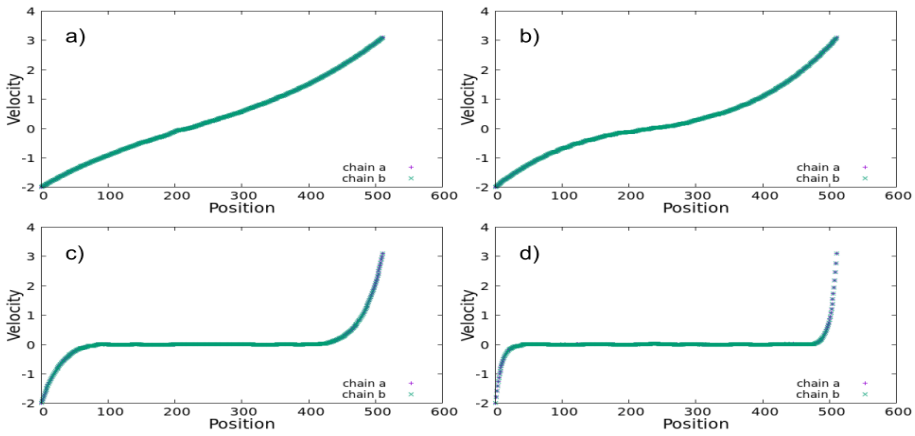


Figure 3.2: Angular velocity versus position in two chain parallel system of 512 rotors under the conditions of Uniform flow regime. $(a)\,\alpha = 0.5$; $(b)\,\alpha = 1.0$; $(c)\,\alpha = 3.0$; $(d)\,\alpha = 3.5$;

- SBR environment at $(T, \mu, \dot{\gamma}) = (0.02{,}10{,}0.007813)$

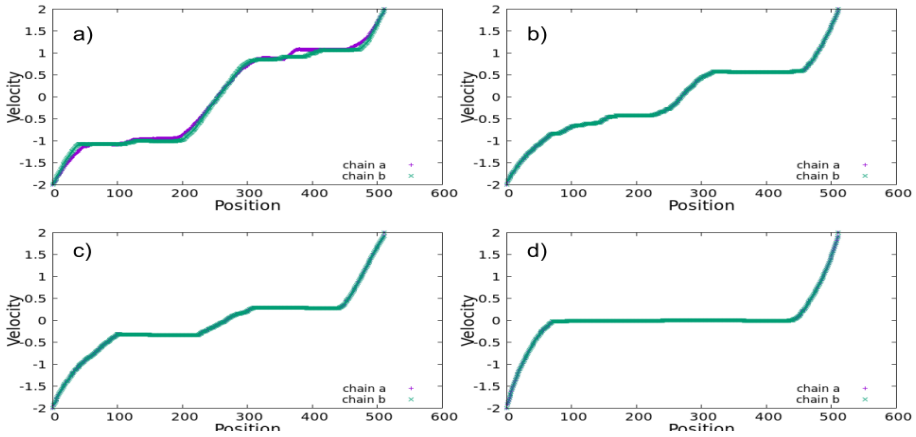


Figure 3.3: Angular velocity versus position in two chain parallel system of 512 rotors under the conditions of SBR. $(a)\,\alpha = 0.00005$; $(b)\,\alpha = 0.5$; $(c)\,\alpha = 1.0$; $(d)\,\alpha = 4.0$;

- Solid-Fluid Coexistence Regime environment at $(T, \mu, \dot{\gamma}) = (0.001{,}1{,}0.0078125)$

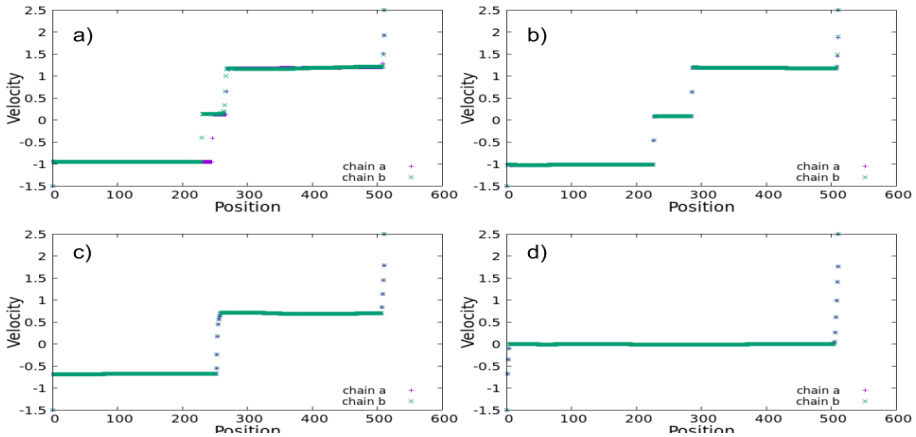


Figure 3.4: Angular velocity versus position in two chain parallel system of 512 rotors under the conditions of Solid-Fluid Coexistence regime. $(a)\,\alpha = 0.0005$; $(b)\,\alpha = 0.05$; $(c)\,\alpha = 2.0$; $(d)\,\alpha = 8.0$;

- Slip Planes Regime environment at $(T, \mu, \dot{\gamma}) = (0.001, 0.5, 0.0058938)$

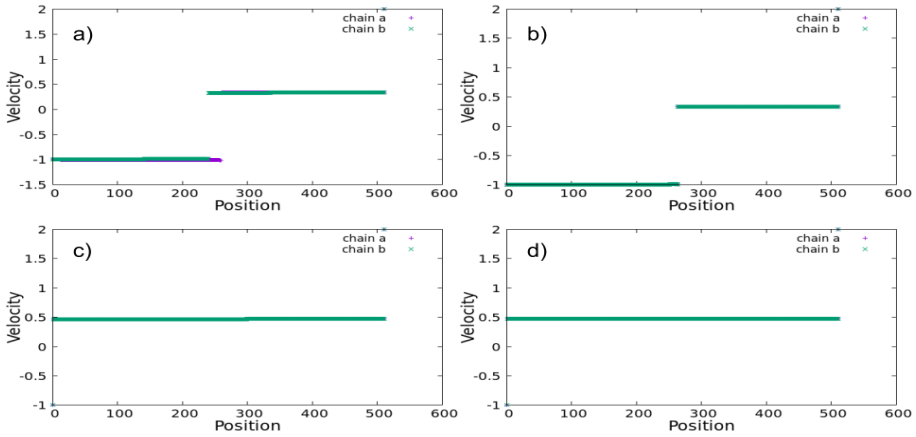


Figure 3.5: Angular velocity versus position in two chain parallel system of 512 rotors under the conditions of Slip Plane regime. $(a)\,\alpha = 0.00005$; $(b)\,\alpha = 0.005$; $(c)\,\alpha = 0.5$; $(d)\,\alpha = 1.0$;

3.2 Perpendicular Two Chain System

3.2.1 Model Description

This is yet another simple XY model consisting of two chain of rotors, but here the orientation of the two chains are different unlike in the previous parallel two chain system. The two chains can be imagined to be placed perpendicular to each other with a single rotor being the only link between the two chains. This common rotor is shared by both the chains as in a junction. As in the previous cases here also the spins only couple to their nearest neighbours. Since there is no interaction between the the chains except through the common rotor, all rotors except the common rotor will have only two interaction terms, which is from its neighbors on either side on the same chain like in the one chain system. As for the common rotor, it will have four interaction terms, two from immediate neighbours on each chain. Like before, the system is spin 1 system. Hamiltonian for the rotors, except for the common rotor, irrespective of the chain in which the rotor belongs to is given by,

$$H = \sum_{j=1}^{N} [-s_j.s_{j-1} + \frac{1}{2}\dot{\theta}_j^2]$$

as usual the first term in the Hamiltonian represent potential energy due to the spin coupling between two neighbour spins and this energy is dependent on the relative orientation between those two specific rotors.The second term represents the rotational kinetic energy of a rotor, which is dependent only on the rotational velocity of that rotor.

Now for the common rotor the Hamiltonian is given by,

$$H = [-s_j^a.s_{j-1}^a - s_j^a.s_{j+1}^a - s_j^b.s_{j-1}^b - s_j^b.s_{j+1}^b + \frac{1}{2}(\dot{\theta}_j)^2]$$

Here the first two terms come from the spin coupling between neighbours present on *chain a*, third and fourth term comes from the spin coupling between neighbours present on *chain b*. These potential energy terms are dependent only on the relative orientation between two rotors. the last term denotes the rotational kinetic energy of the rotor which is dependent on it's angular velocity.

The system is driven out of equilibrium by adding a pair of counter rotating driving rotors on either side of both chains. These rotors are made to rotate at a constant velocity in time and therefore continuously supply energy to the system.

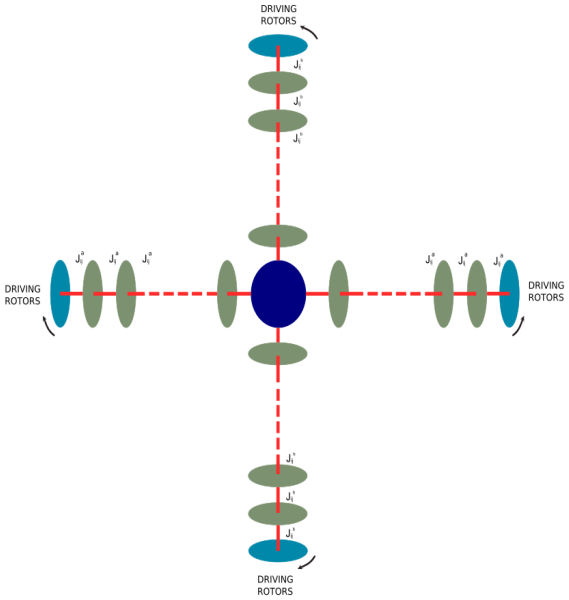


Figure 3.6: Schematic representation of peprendicular two chain XY system. The light blue ellipses at the ends represent counter rotating driving rotors. J_{ij}'s are the intra-chain coupling constant of respective chains. The dark blue circle at the center represents the common rotor.

3.2.2 Model Simulation

Langevin dynamics were applied to develop and study the system. The nature of forces and motion of rotors are same as those in the one chain system. As mentioned before all rotors except the common rotor will have two interaction terms whereas the common rotor will have four. The dynamical equations for the system are as follows,

for all rotors except the common rotor,

$$\ddot{\theta}_j \;=\; \tau_j - \tau_{j-1},$$

for the common rotor,

$$\ddot{\theta}_j \;=\; \tau_j^a - \tau_{j-1}^a + \tau_j^b - \tau_{j-1}^b$$

where,

$$\tau_j \;=\; \sin\Delta\theta_j + \mu\Delta\dot{\theta}_j + \eta_j(t)$$

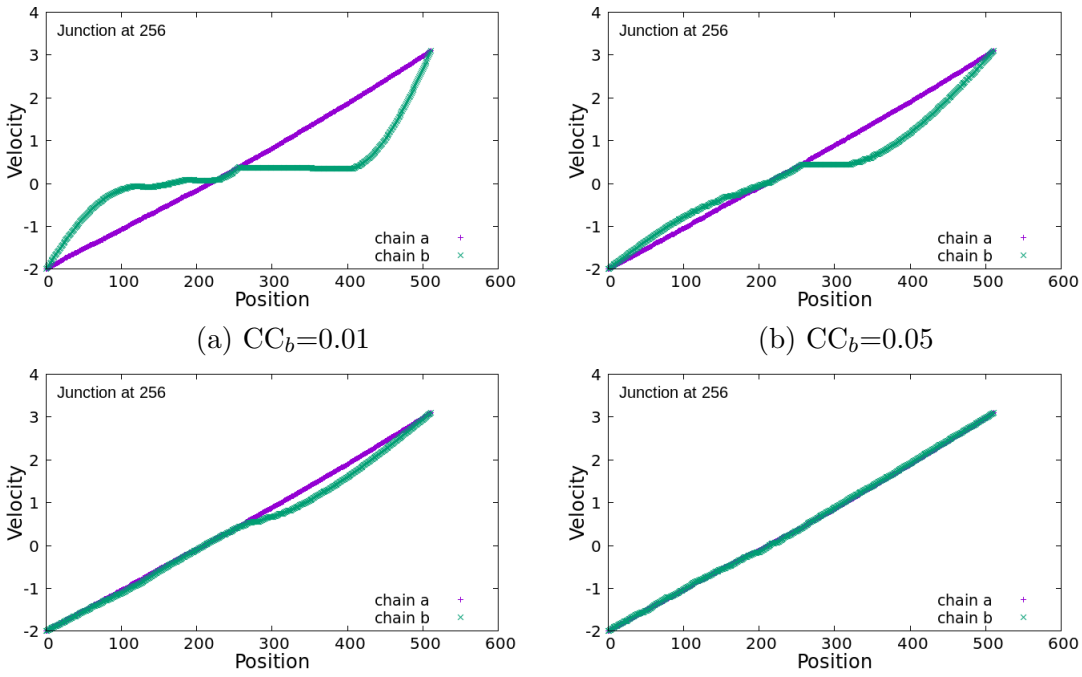
Here, τ_j is the torque applied by rotor $j+1$ on rotor j. $\Delta\theta_j$ is the relative angular difference between rotors at lattice points $j+1$ and j,($\Delta\theta_j \;=\; \theta_{j+1} - \theta j$). μ is the coefficient of friction and $\eta_j(t)$ is the usual δ-correlated Gaussian function with mean zero.

The simulations were done with $k_B \equiv 1$ at a temperature, T and μ was same for all rotors on the same chain, including the driving rotors. Dissipative Particle Dynamics (DPD) algorithm was used to evolve the system. Finite size effect was eliminated by setting the total number of rotors to be $512(N)$ on both chains. An overall global shear rate, $(N\dot{\gamma})$ was applied on the system through the velocity difference between the counter rotating driving rotors making the mean shear rate,

angular velocity difference per rotor, $\dot{\gamma}$. The system variables T, μ, $\dot{\gamma}$ and also the intra-chain coupling of two chains determined the behaviour of the system.

3.3 Results

The model was evolved at different system parameters corresponding to specific flow regimes. The system was evolved for asymptotically late times $t \geq 4500$ and the velocity of rotors were averaged over 500 units of time. The intra-chain coupling of chain b, CC_b was varied with intra-chain coupling of chain a, CC_a kept at unity. This was to study the impact of the common rotor on both chains. The results are shown below.

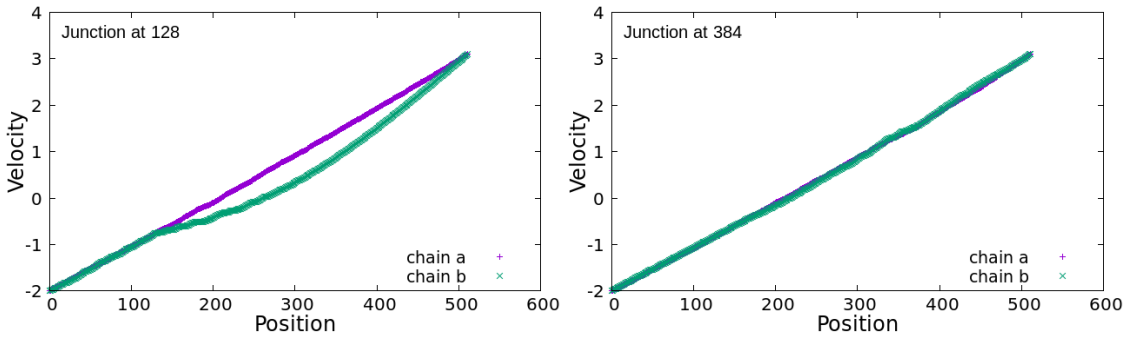


(a) CC_b=0.01 (b) CC_b=0.05

(c) CC_b=0.1 (d) CC_b=0.2

Figure 3.7: Velocity distribution of two perpendicular chain model evolved under uniform regime at T=0.02 and t≥4500. Common rotor at lattice point j=256. Intra-chain coupling constants CC_a=1 for all cases and CC_b is varied

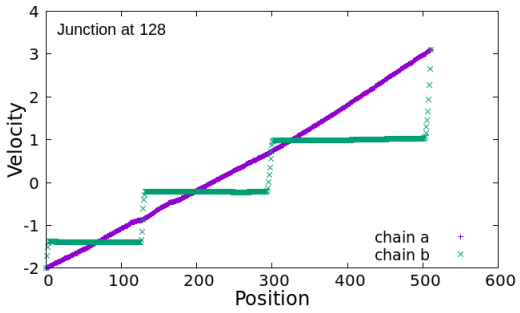
Since the junction of intersection or the position of the common rotor could be anywhere along the chain, it was also varied to see if there was any consequential effect on the behaviour of the system.



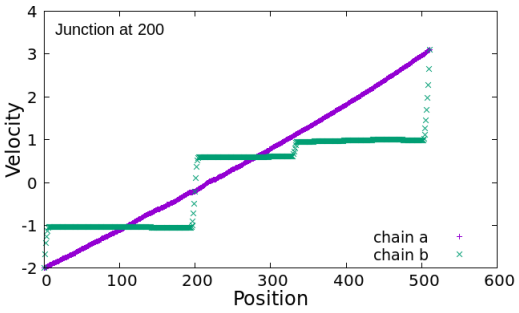
(a) Common rotor at lattice point j=128 (b) Common rotor at lattice point j=384

Figure 3.8: Velocity distribution of perpendicular two chain system evolved under uniform regime at t≥4500. The position of the common rotor is varied. Intra-chain coupling constants CC_a=1 and CC_b=0.1 for both cases

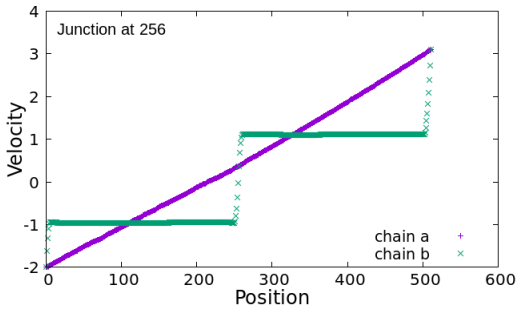
Another interesting operation which was done here was to evolve the two chains under different co-efficient of frictions , μ_1 for *chain a* and μ_2 for *chain b*, but in the same temperature. Since the co-efficient of friction significantly affects the velocity distribution of the rotors and it in turn affects the steady state, we can evolve the chain into a different flow regime under the same temperature by changing μ. This approach cannot be taken in the parallel two chain system since it would be hard to define the inter-chain reaction. The intra-chain coupling constant was chosen to be unity for both the chains. The results are shown below.



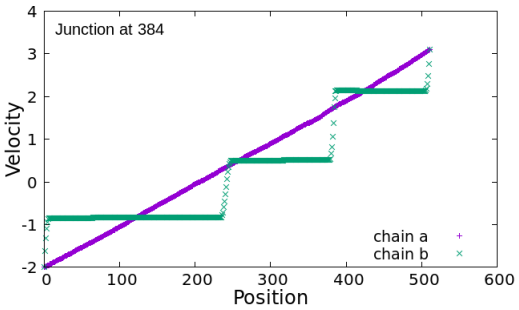
(a) Common rotor at lattice point j=128



(b) Common rotor at lattice point j=200



(c) Common rotor at lattice point j=256



(d) Common rotor at lattice point j=384

Figure 3.9: Velocity distribution of perpendicular two chain system in which *Chain a* is developed under Uniform flow regime conditions and *Chain b* is developed under solid-fluid coexistence regime condition at the same temperature, T=0.02. CC_a=1 and CC_b=1. The position of the common rotor was varied.

Chapter 4

Summary

In this work we started with one of the simplest and basic paradigm of soft condensed matter, one-dimensional XY model to explore its mimicking nature of non-Newtonian fluids. Using Langevin dynamics to develop and study the motion and interaction of rotors present in the chain, we were able to show that the system exhibited different distinct types of angular velocity distribution along the chain for different combination of system parameters signifying different types of shear rate distribution along the layers of a non-Newtonian fluid. The different types of velocity distributions were characterized into four categories, namely, uniform flow regime, SBR, solid-fluid coexistence regime and slip planes regime. To ensure they were in fact steady states the system was developed for much longer time duration and it was observed that the characteristics remained the same.

Later we modified the system by adding one more chain to the one-dimensional XY model. These two chains were aligned parallel and perpendicular to each other and evolved in different flow regime environment to see the impact one had on the other. It was observed that the chains influenced each other more in the parallel two chain system even for very small inter-chain interaction. In the perpendicular two chain system we also developed the two chains under different

fluid flow regimes at the same temperature to see how they responded to such a scenario. On developing one chain in uniform flow regime and the other in solid-fluid coexistence regime, it was observed that the common rotor on the latter chain always positioned itself on the fluid part of the solid-fluid coexistence regime. This suggests that we may be able to dictate the position of fluid part and hence the solid part in a solid-fluid coexistence regime.

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Appendix A

C Program used for 1D XY Model

This is the C program used to develop the datats for 1D XY model.

```
#include <stdio.h>
#include <math.h>
#include "header.h"

double acceleration(int k,double a,double v);
double theta[512],vel[512],avg[512],dt,t,g,T,mu,r,p,q,cc;
long seed;

// Accelereation Function
double acceleration(int k,double a,double v){
  p = sin(theta[k+1]-a) + mu*(vel[k+1]-v) + r*gasdev(&seed) ;
  q = sin(a-theta[k-1]) + mu*(v-vel[k-1]) + r*gasdev(&seed) ;
  return (p-q);
}
```

```
int main()
{
        int c,i,j,k,n,N,tt,nn;
        float th,dx1,dv1,dx2,dv2,dx3,dv3,dx4,dv4,dx,dv;
        FILE *fpr=fopen("tavg1.txt","w");
        seed =-12345;
        N=512;          //Number of Rotors
        tt=450000;      //Time upto which system is evolved
        dt=0.01;        // Time interval
        c=0;
        T=0.02;          //Temperature
        mu=50.;          //Coefficient of friction
        r=sqrt(2*mu*T*dt);

        for(i=0;i<N;i++)       //initial condition----
        {
                theta[i]=M_PI*ran1(&seed);
                vel[i]=0.1*ran1(&seed);
                avg[i]=0;
        }

        t=0;
        vel[0]=-2.;          //Velocity of driving rotors
        vel[N-1]=3.1;
        for(i=0;i<=500000;i++){      //Time loop
            t+=dt;
```

```
    theta[0]+=vel[0]*dt;
    theta[N-1]+=vel[N-1]*dt;

    for(j=1;j<N-1;j++){       // RK-4 Algorithm
        dx1=dt*vel[j];
        dv1=dt*acceleration(j,theta[j],vel[j]);
        dx2=dt*(vel[j]+dv1/2);
        dv2=dt*acceleration(j,theta[j]+dx1/2,vel[j]+dv1/2);
        dx3=dt*(vel[j]+dv2/2);
        dv3=dt*acceleration(j,theta[j]+dx2/2,vel[j]+dv2/2);
        dx4=dt*(vel[j]+dv3);
        dv4=dt*acceleration(j,theta[j]+dx3,vel[j]+dv3);
        dx=(dx1+2*dx2+2*dx3+dx4)/6;
        dv=(dv1+2*dv2+2*dv3+dv4)/6;
        theta[j] += dx;
        vel[j]   += dv;
 }
 if(i==tt-1){           // Averaging velocities
    c++;
    for(k=0;k<N;k++){
        avg[k]+=vel[k];
    }
    tt+=100;
 }
}

for(i=0;i<N;i++){       // Output
```

```
            fprintf(fpr,"%d %f %f \n",i,theta[i],avg[i]/c);
        }
}
```

Appendix B

C Program used for parallel two chain XY Model

This is the C program used to develop the datas for parallel two chain XY Model.

```
#include <stdio.h>
#include <math.h>
#include "header.h"

double acceleration1(int k,double a,double v);
double acceleration2(int k,double a,double v);

double tor[512],theta1[512],theta2[512],vel1[512],vel2[512],
avg1[512],avg2[512],dt,t,ti,g,T,mu,r,p,q,o,s,cc;
long seed;
```

```
int main()
{
        int c,i,j,k,n,N,tt,ttt,nn,jn,NS;
        float th,dx1,dv1,dx2,dv2,dx3,dv3,dx4,dv4,dx,dv;
        FILE *fpr=fopen("quasi7.txt","w");
        seed=-12345;
        N=512;T=0.02;mu=50.0;   //system parameters
        ti=4500;ttt=1000;dt=0.01;
        cc=0.5;       // inter-chain coupling constant;
        tt=floor(ti/dt); // Timepoint at which averaging begins
        NS=floor((ti+500.0)/dt); //No.of time steps required
        r=sqrt(2*mu*T*dt);

        for(i=0;i<N;i++){}    //initial condition----
                theta1[i]=M_PI*ran1(&seed);
                theta2[i]=M_PI*ran1(&seed);
                vel1[i]=vel2[i]=0.;
                avg1[i]=avg2[i]=0.;
        }
        c=0;t=0;

        vel1[0]=-2.;        //Velocity of driving rotors
        vel1[N-1]=3.1;
        vel2[0]=-2.0;
        vel2[N-1]=3.1;
```

```
for(i=0;i<=NS;i++){      //Time Loop
  t+=dt;
  theta1[0]+=vel1[0]*dt;theta2[0]+=vel2[0]*dt;
  theta1[N-1]+=vel1[N-1]*dt;theta2[N-1]+=vel2[N-1]*dt;
  for(j=1;j<N-1;j++){
  //--------------------RK-4 Algorithm for chain a
      dx1=dt*vel1[j];
      dv1=dt*acceleration1(j,theta1[j],vel1[j]);
      dx2=dt*(vel1[j]+dv1/2);
      dv2=dt*acceleration1(j,theta1[j]+dx1/2,vel1[j]+dv1/2);
      dx3=dt*(vel1[j]+dv2/2);
      dv3=dt*acceleration1(j,theta1[j]+dx2/2,vel1[j]+dv2/2);
      dx4=dt*(vel1[j]+dv3);
      dv4=dt*acceleration1(j,theta1[j]+dx3,vel1[j]+dv3);
      dx=(dx1+2*dx2+2*dx3+dx4)/6;
      dv=(dv1+2*dv2+2*dv3+dv4)/6;
      theta1[j] += dx;
      vel1[j]   += dv;
//----------------------RK-4 Algorithm for chain b
      dx1=dt*vel2[j];
      dv1=dt*acceleration2(j,theta2[j],vel2[j]);
      dx2=dt*(vel2[j]+dv1/2);
      dv2=dt*acceleration2(j,theta2[j]+dx1/2,vel2[j]+dv1/2);
      dx3=dt*(vel2[j]+dv2/2);
      dv3=dt*acceleration2(j,theta2[j]+dx2/2,vel2[j]+dv2/2);
      dx4=dt*(vel2[j]+dv3);
      dv4=dt*acceleration2(j,theta2[j]+dx3,vel2[j]+dv3);
```

```
            dx=(dx1+2*dx2+2*dx3+dx4)/6;
            dv=(dv1+2*dv2+2*dv3+dv4)/6;
            theta2[j] += dx;
            vel2[j]   += dv;
          }

          if(i==tt-1){
          c++;
          for(k=0;k<N;k++){
            avg1[k]+=vel1[k];
            avg2[k]+=vel2[k];
          }
          tt+=100;
        }
      }
      for(i=0;i<N;i++){    //Output
         fprintf(fpr,"%d %f %f \n",i,avg1[i]/c,avg2[i]/c);
      }
      fclose(fpr);
}

double acceleration1(int k,double a,double v){ // Chain a
   p = sin(theta1[k+1]-a) + mu*(vel1[k+1]-v) + r*gasdev(&seed) ;
   q = sin(a-theta1[k-1]) + mu*(v-vel1[k-1]) + r*gasdev(&seed) ;
   o = sin(a-theta2[k])   + mu*(v-vel2[k])   + r*gasdev(&seed) ;
   return p-q -cc*o ;
}
```

```
double acceleration2(int k,double a,double v){ //Chain b
   p = sin(theta2[k+1]-a) + mu*(vel2[k+1]-v) + r*gasdev(&seed) ;
   q = sin(a-theta2[k-1]) + mu*(v-vel2[k-1]) + r*gasdev(&seed) ;
   o = sin(theta1[k]-a)   + mu*(vel1[k]-v)   + r*gasdev(&seed) ;
   return p-q+cc*o ;
}
```

Appendix C

C Program used for perpendicular two chain XY Model

This is the C program used to develop the datas for perpendicular two chain XY Model.

```
#include<stdio.h>
#include<math.h>
#include"header.h"

double acceleration1(int k,double a,double v);
double acceleration2(int k,double a,double v);
double acceleration3(int k,double a,double v);

double tor[512],theta1[512],theta2[512],vel1[512],vel2[512],
avg1[512],avg2[512],dt,t,ti,g,T,mu,r,p,q,o,s,cc1,cc2;
long seed;
```

```
int main()
{
        int c,i,j,k,n,N,tt,ttt,nn,jn,NS;
        float th,dx1,dv1,dx2,dv2,dx3,dv3,dx4,dv4,dx,dv;
        FILE *fpr=fopen("quasi7.txt","w");
        seed=-12345;
        N=512;T=0.02;mu=50.0;
        ti=4500;ttt=1000;dt=0.01;
        cc1=1.0;    // intra-chain coupling constants
        cc2=0.1;
        tt=floor(ti/dt); // Timepoint at which averaging begins
        NS=floor((ti+500.0)/dt); //No.of time steps required
        r=sqrt(2*mu*T*dt);

        for(i=0;i<N;i++){}    //initial condition----
                theta1[i]=M_PI*ran1(&seed);
                theta2[i]=M_PI*ran1(&seed);
                vel1[i]=vel2[i]=0.;
                avg1[i]=avg2[i]=0.;
        }
        c=0;t=0;
        jn=256      //Lattice point of Common rotor

        vel1[0]=-2.;        //Velocity of driving rotors
        vel1[N-1]=3.1;
        vel2[0]=-2.0;
```

```
vel2[N-1]=3.1;

for(i=0;i<=NS;i++){     //Time Loop
  t+=dt;
  theta1[0]+=vel1[0]*dt;theta2[0]+=vel2[0]*dt;
  theta1[N-1]+=vel1[N-1]*dt;theta2[N-1]+=vel2[N-1]*dt;
  for(j=1;j<N-1;j++){
    if (j!=jn){          //Not the common rotor
      dx1=dt*vel1[j];    //RK-4 Algorithm for chain a
      dv1=dt*acceleration1(j,theta1[j],vel1[j]);
      dx2=dt*(vel1[j]+dv1/2);
      dv2=dt*acceleration1(j,theta1[j]+dx1/2,vel1[j]+dv1/2);
      dx3=dt*(vel1[j]+dv2/2);
      dv3=dt*acceleration1(j,theta1[j]+dx2/2,vel1[j]+dv2/2);
      dx4=dt*(vel1[j]+dv3);
      dv4=dt*acceleration1(j,theta1[j]+dx3,vel1[j]+dv3);
      dx=(dx1+2*dx2+2*dx3+dx4)/6;
      dv=(dv1+2*dv2+2*dv3+dv4)/6;
      theta1[j] += dx;
      vel1[j]   += dv;
//----------------------RK-4 Algorithm for chain b
      dx1=dt*vel2[j];
      dv1=dt*acceleration2(j,theta2[j],vel2[j]);
      dx2=dt*(vel2[j]+dv1/2);
      dv2=dt*acceleration2(j,theta2[j]+dx1/2,vel2[j]+dv1/2);
      dx3=dt*(vel2[j]+dv2/2);
      dv3=dt*acceleration2(j,theta2[j]+dx2/2,vel2[j]+dv2/2);
```

```
    dx4=dt*(vel2[j]+dv3);
    dv4=dt*acceleration2(j,theta2[j]+dx3,vel2[j]+dv3);
    dx=(dx1+2*dx2+2*dx3+dx4)/6;
    dv=(dv1+2*dv2+2*dv3+dv4)/6;
    theta2[j] += dx;
    vel2[j]   += dv;
  }
  if (j==jn){
    dx1=dt*vel1[j];
    dv1=dt*acceleration3(j,theta1[j],vel1[j]);
    dx2=dt*(vel1[j]+dv1/2);
    dv2=dt*acceleration3(j,theta1[j]+dx1/2,vel1[j]+dv1/2);
    dx3=dt*(vel1[j]+dv2/2);
    dv3=dt*acceleration3(j,theta1[j]+dx2/2,vel1[j]+dv2/2);
    dx4=dt*(vel1[j]+dv3);
    dv4=dt*acceleration3(j,theta1[j]+dx3,vel1[j]+dv3);
    dx=(dx1+2*dx2+2*dx3+dx4)/6;
    dv=(dv1+2*dv2+2*dv3+dv4)/6;
    theta1[j] += dx;
    vel1[j]   += dv;
  }
}
if(i==tt-1){
  c++;
  for(k=0;k<N;k++){
    avg1[k]+=vel1[k];
    avg2[k]+=vel2[k];
```

```
            }
            tt+=100;
          }
        }
        for(i=0;i<N;i++){     //Output
           fprintf(fpr,"%d %f %f \n",i,avg1[i]/c,avg2[i]/c);
        }
        fclose(fpr);
}

double acceleration1(int k,double a,double v){ // Chain a
   p = sin(theta1[k+1]-a) + mu*(vel1[k+1]-v) + r*gasdev(&seed) ;
   q = sin(a-theta1[k-1]) + mu*(v-vel1[k-1]) + r*gasdev(&seed) ;
   return cc1*(p-q) ;
}
double acceleration2(int k,double a,double v){ //Chain b
   o = sin(theta2[k+1]-a) + mu*(vel2[k+1]-v) + r*gasdev(&seed) ;
   s = sin(a-theta2[k-1]) + mu*(v-vel2[k-1]) + r*gasdev(&seed) ;
   return cc2*(o-s);
}
double acceleration3(int k,double a,double v){ //Common Rotor
   p = sin(theta1[k+1]-a) + mu*(vel1[k+1]-v) + r*gasdev(&seed) ;
   q = sin(a-theta1[k-1]) + mu*(v-vel1[k-1]) + r*gasdev(&seed) ;
   o = sin(theta2[k+1]-a) + mu*(vel2[k+1]-v) + r*gasdev(&seed) ;
   s = sin(a-theta2[k-1]) + mu*(v-vel2[k-1]) + r*gasdev(&seed) ;
   return cc1*(p-q)+cc2*(o-s);
}
```