Active Matter

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Certificate of Examination

This is to certify that the dissertation titled **Active Matter** submitted by **Garima Singh** (Reg. No. MS11012) 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.

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Dated: April 22, 2016

Declaration

The work presented in this dissertation has been carried out by me under the guidance of Dr. Abhishek Chaudhuri 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.

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

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Acknowledgment

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Abstract

The aim of the project is to understand active systems and model them subsequently. In active matter, particles use stored or ambient energy to perform systematic movement. To quantify the dynamical organization of active matter , we review agent based models (Vicsek) as well as coarse grained hydrodynamic description (Toner-Tu) of these systems. We also review lquid crystal physics to better understand the liquid crystalline orders observed in active matter. We then discuss a stochastic lattice gas model which successfully describes an active system.

Contents

Chapter 1

Active Matter

1.1 Active Matter

What is active matter? It is a collection of particles, units and entities which are individually driven so there is a drive that acts on each unit and collectively they generate coordinated motion at large scales[MJR+13, Ram10, Ton15, Mar15]. The key here is that it is a non equilibrium system. Drive is internally generated on these active particle generally through an internal cyclic transformation for instance chemical energy . An example could be a bacterium which beats the flagella which undergoes a cyclic transformation and swims.This type of motion has profound consequences in collective behaviour.Such sytems may exhibit collective swarming, turbulence , vorticity and may organise in regular periodic patterns depending on situations. Many examples of active system comes from living world. One of the reason for such kind of collective motion could be protection from predator, availability of food, etc.

Examples of such system:

1. Inside a cell: cytoskeleton $\rightarrow$ cell motility, division, mechanics etc.

2. Group of cells $\rightarrow$ tissues, mechanics, collective migration, wound healing , etc.

3. Fish , birds, people , etc.

4. Synthetic microswimmer

What do all these have in common? All of these are individually driven, undergoes symmetry breaking locally and undergoes order/disorder transition.They show liquid crystalline order and can be called active liquid crystals. We will review liquid crystals in the

next chapter.

We will use methods from statistical mechanics and soft condensed matter to understand which new states of active matter are possible. Is it possible to classify behaviours and identify generic properties. What is the order parameter to change from one state to another. We will start be classifying them on the basis of types of orientational order.

Types of Orientational Order:

1. Polar : Examples - Bacteria, fish, etc. The particles have head and tail and can distinguish between the two. When in high density can order with same symmetry as ferromagnetic or polar order. The order parameter will be a vector. If we assign a unit vector $\hat{v}_i$ to each individual we can define a polarization field as $P = \langle \sum_i \hat{v}_i \delta(r - r_i) \rangle$. This is a continuum field which describe average orientation of particle. P is also proportional to the mean velocity of the system so this quantity P play a dual role as polarization and velocity. What are the consequences of this dual role. The order state has a non-zero mean motion

2. Apolar : System which has no head and tail and are symmetric and may go around back and forth. Order is similar to that of nematic liquid crystal. Here the order parameter will be a tensor. These system do not exhibit any mean motion.

3. Spherical colloids : Which might be self propelled and unless there is an external imposed rule that tends to align them, they do not align because of steric hindrances. They do not exhibit orientational order but shows rich non-equilibrium behaviour.

Polar particles can align in nematic state when half are going in one direction and other half in other. But no living system exhibit this kind of behaviour.

Distinguishing between medium: If the medium only provides friction then it is dry. If the medium provides hydrodynamic interaction then its wet. Can be imagined as active particle in a suspension/fluid. The velocity of the fluid could be different from that of active particles.

There is a lot of work been done in agent based model of active matter where we consider them as point particles which tends to align following certain rule.

1.1.1 From Vicsek to Continuum

This is inspired by analogy with ferromagnetism. Its of the first variety i.e. the polar system. In 2D it is similar to flying XY spins. These are point particles and each particle is described by fixed speed v_0 and orientation $\hat{e}_i$ which makes an angle θ_i. So $\hat{e}_i = (cos\theta_i, sin\theta_i)$. The dynamics is overdamped that means it has friction. They align in the average direction of

neighbours in the radius r with some noise . The position after some time $\triangle t$ will be

$$\vec{r}_i(t + \triangle t) = \vec{r}_i(t) + v_0\hat{\mathsf{e}}_i\triangle t \tag{1.1}$$

$$\theta_i(t + \triangle t) = \langle\theta_i(t)\rangle_R + \eta_i(t) \tag{1.2}$$

η_i is random noise uniform in $\left[-\frac{\eta}{2}, \frac{\eta}{2}\right]$. So the parameter of the model is strength of noise and density. We can define an order parameter to be $v = \left|\frac{1}{N}\sum_i \vec{v}_i(t)\right|$ where $\vec{v}_i = v_0\hat{\mathsf{e}}_i$. On simulation it shows that it exhibit a phase transition as a function of strength of noise and density. This is a first order phase transition. At low noise or high density there is order so the motion is in same direction whereas at high noise or low density there is disorder and everyone is moving haphazardly. There is breaking up of continuum symmetry in 2D. In equilibrium it would have been impossible because of Mermin-Wagner theorem but in non-equilibrium system like this it can happen. **Mermin-Wagner theorem** states that continuous symmetry cannot be spontaneously broken at finite temperature in systems with sufficiently short range interactions in dim $d \leq 2$.

For equilibrium system we have free energy and therefore, we can relate the dynamics to derivatives of free energy. But for these non-equilibrium system we don't have free energy so we can write such equations on the basis of very general rules such as symmetry consideration, conservation laws, etc . This method gives you equation which are generic and does not depend on specific system. On the other hand all the parameters are unknown as we are out of equilibrium and there is no constraint like fluctuation dissipation that relates various parameter in equilibrium.

We will study the continuum version of the model as we are observing over larger length and time scale which is the field theory and is also known as Toner-Tu model. We will start with microscopic model and derive Toner-Tu equation which is the continuum version of Vicsek model. But before that we review Langevin and Smoluchowski dynamics of a particle in a bath.

1.1.2   From Langevin dynamics to Smoluchowski

$$m\frac{d\vec{v}}{dt} = -\zeta\vec{v} + \vec{\eta}(t) \tag{1.3}$$

We can write the above Langevin equation for a brownian particle[Bha07]. This is just a F=ma type of equation. The first term on the write describe drag which is the mean effect of collision with the fluid and the friction coefficient ζ if this is a spherical brownian particle which has stokes form i.e. $\zeta = 6\pi\eta a$ where η is the shear viscosity of the fluid and

'a' is the radius of the colloid. This expression is in 3D. And $\vec{\eta}(t)$ is a random force and is supposed to describe the random part of the collisions with fluids and we define this random force or noise in terms of its moments. We can choose it to be Gaussian and white i.e. $\langle \vec{\eta}(t) \rangle = 0$ and delta correlated in time i.e. collisions are uncorrelated $\langle \eta_i(t) \eta_j(t') \rangle = 2\Delta \delta_{ij} \delta(t - t')$. There is a characteristic time scale in this equation $\tau = \frac{m}{\zeta}$ and it describes competition between inertia and viscous drag. d-dimensionality, Δ- noise strength or correlator of noise, ζ-friction, m-mass of particle. We can define equal time correlator of velocity which we can exactly calculate and look at time much larger than $\frac{m}{\zeta}$

$$\left\langle [\vec{v}(t)]^2 \right\rangle \xrightarrow[t >> \frac{m}{\zeta}]{} \frac{\Delta d}{\zeta m} \underset{equilibrium}{=} \left\langle v_{th}^2 \right\rangle = \frac{d k_B T}{m} \tag{1.4}$$

If we define brownian particle in a fluid in thermal equilibrium then after long time the system is in equilibrium then we can calculate $\left\langle [\vec{v}(t)]^2 \right\rangle$ from the distribution of the velocity in the system which is expected to be Maxwellian.

We can also calculate the mean square displacement

$$\left\langle [\Delta \vec{r}(t)]^2 \right\rangle = 2d \frac{k_B T}{\zeta} \left\{ t - \tau(1 - e^{-\frac{t}{\tau}}) \right\} \tag{1.5}$$

where $\Delta \vec{r}(t) = \vec{r}(t) - \vec{r}(0)$. Assuming system is in equilibrium.

$$t << \tau \qquad \left\langle [\Delta \vec{r}(t)]^2 \right\rangle = d \frac{k_B T}{m} t^2 \text{ ballistic} \tag{1.6}$$

$$t >> \tau \qquad \left\langle [\Delta \vec{r}(t)]^2 \right\rangle = 2Ddt \text{ diffusive} \tag{1.7}$$

where $D = \frac{k_B T}{\zeta}$ is Einstein relation which relates diffusion to friction. In ballistic case displacement goes linearly with time. We were interested in $t >> \frac{m}{\zeta}$ so we could have neglected inertia as compared to drag which is an overdamped limit $t >> \tau$. So we can write our equation of motion as

$$\zeta \vec{v} = \vec{\eta}(t) \tag{1.8}$$

So we can calculate the mean square displacement and find the diffusive behaviour. Now imagine that there are many particles and we have to write coupled Langevin equation. This is fine when we have to do numerical dynamic simulations but analytically this is not very useful. Therefore, we need to do some coarse graining. So, instead of writing Langevin equation we will describe the system in probability distribution for a particle to be at some position at time t. That is known as Smoluchowski equation. And we will further coarse grain that because we are interested in large length and time scale then we should describe system in terms of fields that relaxes slowly eg. fields related to broken symmetry. We will try to do it in 1D and find an equation for noise averaged probability distribution $\psi(x,t)$ to find a particle at position x at time t. We will assume overdamped

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dynamics. So the equation of motion can be written as

$$v = \frac{dx}{dt} = \tilde{\eta}(t) - \frac{1}{\zeta}U'(x) \tag{1.9}$$

In order to keep a track of external forces as eventually we will deal with interaction with other particles we will keep possible external force derived from external potential . Noise is again gaussian and white i.e $\langle \vec{\eta}(t) \rangle = 0$ and delta correlated in time i.e. collisions are uncorrelated $\langle \eta(t)\eta(t') \rangle = 2\Delta\delta(t - t')$.

$\hat{\psi}(x,t)$ in 1D is not yet noise averaged. Since the number of particle is conserved so the probability density is conserved and so,

$$\int_V dx \hat{\psi}(x,t) = 1 \tag{1.10}$$

This implies , conservation law for the probability and that implies time derivative of probability is gradient of flux. Flux is velocity times probability density.

$$\partial_t \hat{\psi} = -\partial_x v \hat{\psi} \tag{1.11}$$

If we substitute the Langevin equation and write the expression of probability density in the following way

$$\partial_t \hat{\psi} = -\partial_x \left[-\frac{1}{\zeta}U'\hat{\psi} \right] - \partial_x \left(\eta\hat{\psi} \right) \tag{1.12}$$

$$\partial_t \hat{\psi} = -L\hat{\psi} - \partial_x \left(\eta\hat{\psi} \right) \tag{1.13}$$

We can now write the formal solution of these equation .

$$\hat{\psi}(t) = e^{-Lt}\hat{\psi}(s) - \int_0^t ds e^{-L(t-s)}\partial_x \left(\eta(s)\hat{\psi}(s) \right) \tag{1.14}$$

Note, $\hat{\psi}(t)$ only depends on noise at time $s < t$. Therefore,

$$\partial_t \hat{\psi} = -L\hat{\psi} - \partial_x \eta(t)e^{-Lt}\hat{\psi}(0) + \partial_x \int_0^t ds \eta(t)e^{-L(t-s)}\partial_x(\eta(s)\hat{\psi}(s)) \tag{1.15}$$

Noise average and let $\psi = \langle \hat{\psi} \rangle$

$$\partial_t \left\langle \hat{\psi} \right\rangle = -\left\langle L\hat{\psi} \right\rangle - \left\langle \partial_x \eta(t)e^{-Lt}\hat{\psi}(0) \right\rangle + \partial_x \left\langle \int_0^t ds \eta(t)e^{-L(t-s)}\partial_x(\eta(s)\hat{\psi}(s)) \right\rangle \tag{1.16}$$

We assume $\hat{\psi}(0)$ does not depend on noise. So the second term on RHS will become zero. $\hat{\psi}$ does depends on noise . Iterating the solution many times and keeping and generating many factors of noise everytime and since the noise is Gaussian , all the powers of noise will be zero on averaging and only even power will contribute for which we can use Wick's

theorem to factorise this and relate all the even powers to second moment. We can contract η's.

After doing this we will end up with Smoluchowski equation.

$$\partial_t \psi = -\partial_x \left[-\frac{1}{\zeta} U' \psi - \Delta \partial_x \psi \right] \tag{1.17}$$

This is the equation for noise averaged probability density for one brownian particle. In equilibrium the second term on RHS will be diffusion coefficient i.e. diffusion times second derivative of density . First term on RHS is mean force time density so this flux that comes from mean force on particles and second term when fluctuation dissipation theorem holds $\Delta = D$. This is Smoluchowski equation and for $U' = 0$ we can find solution.

We will now try to get a hydrodynamic description of active matter. Describe large scale dynamics in terms of a small number of continuum fields that are 'slow' $\longrightarrow$ field theory $\omega(k) \to 0$, $\lambda \to \infty$.[Mar15]

Derivation of Toner-Tu equation

We will start with continuous time version of Vicsek model where point particle are self propelled with velocity v_0 in the direction $\hat{e}$ and align with neighbours with rate γ with rotational noise of the rate D_r. Neglecting translational thermal noise,

$$\frac{d\vec{r_i}}{dt} = v_0 \hat{e}_i \tag{1.18}$$

Rotational evolution equation has noise.

$$\frac{d\theta_i}{dt} = \gamma \Sigma_j F(\theta_i - \theta_j, \vec{r}_j - \vec{r}_i) + \sqrt{2Dr}\eta_i(t) \tag{1.19}$$

D_r is strength of noise. $\eta_i \epsilon \left[-\frac{1}{2}, \frac{1}{2} \right]$

F describes the interaction and we will chose in a very simple form as it is a short range interaction.

$$F(\theta_i - \theta_j, \vec{r}_j - \vec{r}_i) = \frac{sin(\theta_j - \theta_i)}{\pi R^2} \; r_{ij} < R \tag{1.20}$$

$$= 0 \text{ otherwise} \tag{1.21}$$

Now, $\psi = \psi(\vec{r}, \theta, t)$ which is one particle probability density. Here we have one more degree of freedom and so we will derive again the Smoluchowski type equation to get

$$\partial_t \psi = -\vec{\nabla}.(v_0 \hat{e} \psi) - D_r \partial_\theta^2 \psi - \gamma \partial_\theta \int d\theta' \int dr' F(\theta' - \theta, \vec{r'} - \vec{r}) \psi(\vec{r'}, \theta', t) \psi(\vec{r}, \theta, t) \tag{1.22}$$

$F(\theta' - \theta, \vec{r'} - \vec{r}) = sin(\theta' - \theta)\delta(\vec{r} - \vec{r'})$ because we are interested in length scale larger than interaction.

$$\partial_t \psi = -\vec{\nabla}.(v_0 \hat{e}\psi) - D_r \partial_\theta^2 \psi - \gamma \partial_\theta \int d\theta' sin(\theta' - \theta)\psi(\vec{r}, \theta', t)\psi(\vec{r}, \theta, t) \qquad (1.23)$$

We can define angular fourier transform

$$\psi_k(\vec{r}, t) = \int \frac{d\theta}{2\pi} e^{ik\theta}\psi(r, \theta, t) \qquad (1.24)$$

$$\psi_0 = \rho \qquad (1.25)$$

$$\psi_1 = \rho(P_x + iP_y) \qquad (1.26)$$

$$\psi_2 = \rho(Q_{xx} + iQ_{xy}) \qquad (1.27)$$

We want to write equation for continuum fields like density which is defined by first angular moment of ψ, polarization density is defined by second angular moment, and so on. We can define ψ in infinite set of moment so we need to do truncation.

$$\rho(\vec{r}, t) = \int \frac{d\theta}{2\pi}\psi \qquad (1.28)$$

$$\rho\vec{P} = \int \frac{d\theta}{2\pi}\hat{e}(\theta)\psi = \vec{w} \qquad (1.29)$$

$$\rho Q_{\alpha\beta} = \int \frac{d\theta}{2\pi}\left(\hat{e}_\alpha \hat{e}_\beta - \frac{1}{2}\delta_{\alpha\beta}\right)\psi \qquad (1.30)$$

ρ defined as first angular moment of ψ, polarization density $\rho\vec{P}$ or $\vec{w}$ is the second angular moment which is also the order parameter, $Q_{\alpha\beta}$ is a symmetric traceless tensor and is the order parameter for nematic system which is also the third angular moment. ψ can be defined as infinite number of moments orthogonal to each other. Density decays slowly so at long wavelength it is a conserved quantity. Polarization is the order parameter of the system and becomes non-zero where orientation of symmetry is sponateously broken so we expect this quantity to decay slowly near phase transition. We want to find continuum hydrodynamic equation for these two fields. All the other moments are fast fields and decay on microscopic timescale of the order of $\frac{1}{D_r}$.

Equation for $\psi(\vec{r}, t) \rightarrow$ infinite set of equations ψ_k which is the kth moment

$$\partial_t \psi_k + \frac{v_0}{2}\partial_x(\psi_{k+1} - \psi_{k-1}) + \frac{v_0}{2i}\partial_y(\psi_{k+1} - \psi_{k-1}) = -k^2 Dr\psi_k + \frac{i\gamma k}{2\pi}\sum_s \psi_s F_{-s}\psi_{k-s} \quad (1.31)$$

For $k = 0$,

$$\partial_t \psi_0 + \frac{v_0}{2}(\partial_x - i\partial_y)\psi_1 = 0 \qquad (1.32)$$

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Then

$$\partial_t \rho = -\vec{\nabla}.(v_0 \rho \vec{P}) \tag{1.33}$$

$\psi_0 \sim \rho$ is a conserved field decaying on hydrodynamic time scale[Kar07]. $\psi_1 \sim \vec{P}$ order parameter decay slowly near phase transition. $\psi_2 = 0$ as they are fast variable decaying at rate D_r so we can neglect ψ_2. So we can assume $\psi_k = 0, k \geq 3$.

So, now we will get two equations for ρ and $\vec{P}$ which are[MJR$^+$13, Ram10]

$$\partial_t \rho = -\vec{\nabla}.(v_0 \vec{w}) \tag{1.34}$$

$$\partial_t \vec{P} + \lambda_1 (\vec{P}.\vec{\nabla})\vec{P} = -\left[\alpha(\rho) + \beta P^2\right]\vec{P} - \frac{v_0}{2}\vec{\nabla}\rho + \frac{\lambda_3}{2}\vec{\nabla}P^2 + \lambda_2 \vec{P}(\vec{\nabla}.\vec{P}) +$$
$$K_3 \nabla^2 \vec{P} + (K_1 - K_3)\vec{\nabla}(\vec{\nabla}.\vec{P}) \tag{1.35}$$

All parameters given in terms of Dr, γ, v_0, ρ_0. First term on RHS is non-linear friction and can be written as $-\frac{1}{\gamma}\frac{\delta F}{\delta \vec{\rho}}$. The expression for F can be written as

$$F = \int_{\vec{r}} \frac{\alpha}{2}\rho^2 + \frac{\beta}{4}\rho^4 \tag{1.36}$$

where,

$$\alpha(\rho) = D_r - \frac{1}{2\pi}\gamma\rho \tag{1.37}$$

$$\beta = \frac{\gamma^2 \rho^2}{32 Dr \rho^2} \tag{1.38}$$

which gives a continuous phase transition where α changes sign at a particular density or a particular value of rotational noise. If $\alpha > 0$ then if we plot F vs P there is one minima at $P = 0$ which is a disordered phase and if $\alpha < 0$ we have 2 minima at finite value of P which is ordere state where $P^2 = -\frac{\alpha}{\beta}$ which is the flocking state or ordered state which is a low noise or high density state.

1.2   Breakdown of Mermin Wagner

Flocking is when large number of things that are self propelled and are moving in same direction . Often these things are living creatures. More generally the details of the organism doesn't matter and only things that are important is the organism at one corner cannot see and interact with the one far away at some other portion of the flock. Secondly, their motion is in one particular direction and is obtained by following the neighbours which the individual can see in immediate vicinity. This can be seen in Fig.(1.1) Nonetheless they are moving in same direction. Therefore, the interaction is short ranged
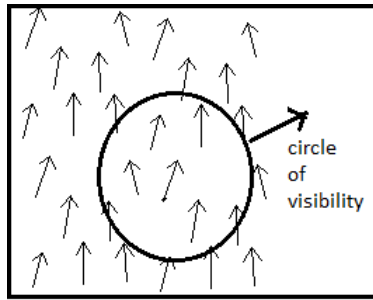
Figure 1.1: Circle of visibility

but order is long ranged . The direction they are picking to move is chosen by the flock and not imposed externally. There is spontaneously broken symmetry . It is astonishing to observe such a behaviour. The theory works equally well for 2 or more dimensions. Flocking is a situation when moving organism continuously and spontaneously break symmetry . In this case the continuous symmetry is rotation invariance. This happening in 2-D is baffling.

Using Mermin-Wagner theorem which says such phenomenon, that is continuously breaking of symmetry in 2-D with only short ranged interaction is impossible. So how is this happening. The point to be noted is in Mermin-Wagner theorem is that it works for systems in equilibrium. But self propelled organisms are out of equilibrium. So, Mermin-Wagner theorem doesn't apply. Now the question arises that what aspect of this non-equilibrium makes it possible for long ranged order in 2D with only short ranged interaction. The important aspect is that these creatures are moving. There is a phenomenon called breakdown of linearized hydrodynamics. For 2D system this is absolutely crucial to have flocking as can be seen in Fig.(1.2). This breakdown of linearized hydrodynamic stabilize the long range order. Short range interaction is whose range is very small as compared to the size of the system under consideration. All these theorem applies when the size of the system goes to infinity or the thermodynamic limit. So any system with finite range interaction if made big enough will fall in this limit. The argument also applies when the interaction goes to infinite distance but the strength falls sufficiently rapidly with distance.[Ton15]

1.2.1 Microscopic Model: Vicsek (2D)

Each creature is a point carrying a vector which will determine its direction of motion. And all of them have synchronised timer and after every time iteration they identify their neighbour and try to follow them by taking average . And move with a speed v_0 which is same for all. A random error is introduced for every iteration while adopting the average motion of neighbours which is taken as a white noise. The error also has zero mean and no
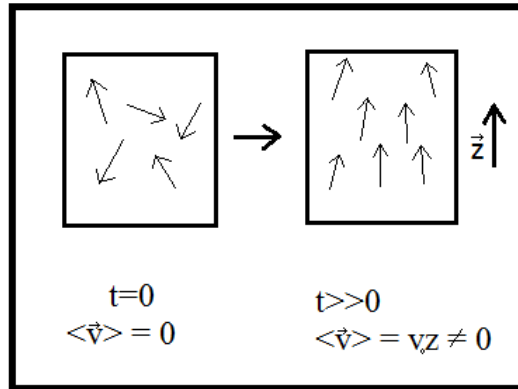
Figure 1.2: Flock sponaneously orders
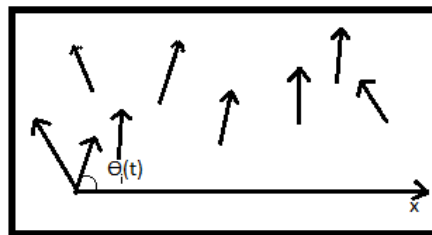
Figure 1.3: Measuring θ for the pointer

memory of past. The question is if the organisms are making mistake and is the system robust against those mistake to have long range order ?

In 2D in the presence of noise this is impossible as it violates the Mermin-Wagner theorem. If instead of moving every particle just point in such a way that everyone tries to point according to the neighbours . Everyone ends up pointing in different direction because of the fluctuation and is of the order of system size. Even if the fluctuation was small , the error is big. And there is no long range order. This is similar to vicsek model except for the particles donot move or velocity is tending to zero. With the same range of interaction , same noise strength but introducing the sole modification that in addition to pointing the particle also move then it works. What is the reason? Why motion makes it possible? In less than 2 D the error accumulate faster then they dissipate. No motion means they are at equilibrium and so Mermin-Wagner theorem applies.

To understand why motion makes it possible to dissipate error faster than accumulation we need to look at slow diffusive process. Let θ be the angle made by the pointer as shown in Fig.(1.3).

Figure 1.4: A 2D lattice

$$\theta_i(t+1) = \langle \theta_j(t) \rangle_{j \in O} + \eta_i(t) \tag{1.39}$$

$$\langle \eta_i \rangle = 0 \tag{1.40}$$

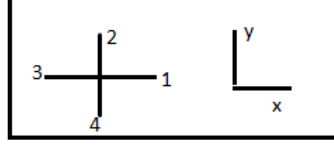$$\langle \eta_i(t)\eta_i(t') \rangle = \Delta \delta_{i,j} \delta_{t,t'} \tag{1.41}$$

$$\tag{1.42}$$

.Rewriting evolution rule : Subtracting $\theta_i(t)$ from both sides.

$$\theta_i(t+1) - \theta_i(t) = \langle \theta_j(t) \rangle - \theta_i(t) + \eta_i \tag{1.43}$$

In the continuum limit,

$$\partial_t \theta = D \left(\partial_x^2 \theta + \partial_y^2 \theta \right) + \eta \tag{1.44}$$

To get an idea how we got this, let us consider a lattice as seen in Fig.(1.4):

$$
\begin{aligned}
\langle \theta_j \rangle - \theta_i &= \frac{1}{4}(\theta_1 + \theta_2 + \theta_3 + \theta_4) - \theta_i && \text{(1.45)} \\
&= \frac{1}{4} \left[(\theta_1 - \theta_i) - (\theta_i - \theta_3) + (\theta_2 - \theta_i) - (\theta_i - \theta_4) \right] && \text{(1.46)} \\
&= \frac{1}{4} \left[\partial_x \theta(x,y) - \partial_x \theta(x-1,y) + \partial_y \theta(x,y) - \partial_y \theta(x,y-1) \right] && \text{(1.47)} \\
&= \frac{1}{4} \left[\partial_x(\partial_x \theta) + \partial_y(\partial_y \theta) \right] && \text{(1.48)}
\end{aligned}
$$

Therefore , we can write this as

$$\partial_t \theta = D \, \nabla^2 \theta + \eta \tag{1.49}$$

This is a diffusion equation.
Properties:

1. Slow : The diffusion equations are slow . We can quantify how slow is the diffusion equation by power counting as shown in Fig.(1.5). Θ over time goes as θ over $(distance)^2$. So that $(distance)^2$ goes as as time and distance as $\sqrt{time}$ as shown in Fig.(1.6).

$$\frac{\theta}{t} \sim \frac{\theta}{x^2} \implies x^2 \propto t \implies x \propto \sqrt{t} \tag{1.50}$$
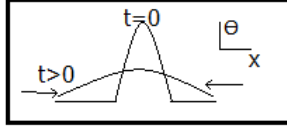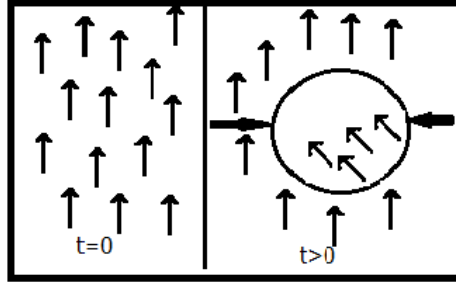
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Figure 1.5: Diffusion with respect to time

Figure 1.6: Diffusion translating outwards to distance proportional to $\sqrt{t}$

2. Conserved : The angles diffuse very slowly through collection of pointers. It conserves the volume integral of whatever its diffusing. Taking volume integral on both sides so the RHS on ignoring the noise is equal to the surface integral. If the surface is far away then we have periodic boundary condition or surface to volume ratio is negligible so can be neglected. Then the total integral of the field in this case the angle of all space doesn't change over time. So its conserved.

$$\int \partial_t \theta d^d r = D \int \triangledown^2 \theta d^d r = D \int \vec{\triangledown}\theta.dS \tag{1.51}$$

$$\int \vec{\triangledown}\theta.d\vec{S} = 0 \tag{1.52}$$

if flock size $>> \sqrt{t}$

Decay at one error: Lets consider what would happen if you turn off the noise in viscek algorithm. Then we will have something that will really favour order. Start with initial condition where everybody is pointing in same direction except one . The individual at the centre is pointing off by some angle θ_0 . Now , if we let the algorithm run for time t. This error will diffuse to distance proportional to $\sqrt{t}$. So , now everybody within the distance equal to $\sqrt{t}$ will also be going to make a mistake. In the first step he is pointing in the direction of neighbour as that iis the average but by then he has contaminated all his neighbours which are off by some angles and this will spread out. In much later time the error has infected everybody in the distance of the order proportional to $\sqrt{t}$ of the original error maker . The error became smaller because the volume integral of the angle is the sum of the angle of all the individuals and that is conserved. So the original error θ_0 is now going to spread over all the individuals within the circle. Evenly divided among them all.

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So the angle of error that anyone is going to make is going to be roughly the original angle θ_0/(number of individual in the circle). If the density is roughly uniform then the number of individual are going to grow with the $(radius)^d$ where d is the dimension of the system under consideration.

$$\theta(t) \approx \frac{\theta_0}{N} \approx \frac{\theta_0}{t^{d/2}} \tag{1.53}$$

Meanwhile, more errors : Total error at center

$$\sqrt{\delta\theta_0^2} = \frac{\sqrt{r_0^d t_0}}{r_0^d} \tag{1.54}$$

r_0 is number of error committers and t_0 of errors each makes. $Error \propto \frac{1}{r^d}$ and $r \propto \sqrt{t}$. Then the error is falling off as $\frac{1}{t^{\frac{d}{2}}}$ .It depends on the dimension of space. As we go to lower dimension this fall off becomes slower and slower and that's why its harder to order a low dimension system than to order a high dimension system. Secondly, its slow. Its not falling off exponentially or fast so there is no characteristic time after which all the error will go away. Its falling off like a power law and that will become smaller as we go down in dimensions. As we reach $d = 2$ its falling as $\frac{1}{t}$ which is very slow indeed. So, what will happen in Vicsek model where errors are trying to decay by very slow process and more errors are constantly being created. We will find that in high enough dimension this decay of error can compete with accumulation of noise and actually suppress accumulation of errors and we can have long range order. But in low enough dimensions you can't . Outside the surface all the angles are uniformly aligned as the error has not reached there so the gradient of the angle is zero. And will remain zero until that region goes out to the boundary of the system. Right now everything is about pointers and not movers. Because the angle field is described by this diffusion equation the error that you make diffuse very slowly.

$$t_0 \sim r_0^2 \implies \delta\theta_0^2 \sim r_0^{2-d} \tag{1.55}$$
$$\delta\theta_1^2 \sim (2r_0)^{2-d} = \delta\theta_0^2 2^{2-d} \tag{1.56}$$

Now we will see what happens when we turn the noise back on. Lets consider a flock of radius r. We have seen that in diffusion equation any errors you make inside this flock will be conserved until enough time has passed such that that error has diffused all the way to the boundary. So any noise generating particle inside the region of radius r can only start to decay on the time it takes for the errors to diffuse all the way to the $boundary \propto (size\ of\ system)^2$. In that time how many errors are made inside this collection of pointers. Each individual pointer makes error on every single time step . So

the number of error made by each pointer goes by time or $radius^2$. So, the total number of error made is the product of the number of pointer (r^d) and error made by each pointer (r^2). So once again dimension of space becomes essential . So,the total number of error becomes r^{d+2}. What is the sum of all these errors ? There is going to be a residual error although some errors will cancel the others. So the typical size of that is the root mean squared error which scales as $\sqrt{total\ error}$. So the error per pointer goes like $\sqrt{total\ error}/(Number\ of\ pointer)$. This ratio will give the typical angular error that each individual pointer is making. Therefore,

Diffusion time $t_D(r) \propto r^2$

Number of errors/pointer $\propto t_D \propto r^2$

Number of pointer $N \propto r^d$

$\implies$ Number of errors $\propto N t_D \propto r^{d+2}$

$\implies$ RMS error/pointer $\delta\theta \propto \frac{\sqrt{r^{d+2}}}{r^d}$

When $d > 2$ and the size of system goes to infinity the error per pointer goes to zero. This means the system is going to be ordered . And when $d < 2$ the error per pointer will go to infinity and so we cannot have a long range order for this case. And $d = 2$ is the marginal case when the error goes as logarithm of the radius and this goes to infinity. So, again no long range order. So thats the justification for Mermin-Wagner theorem which says that you cannot have long range order for $d \leq 2$ because the error accumulate faster than it can be dissipated as they can only be dissipated by this slow diffusive process in equilibrium.

$$\delta\theta \propto r^{1-\frac{d}{2}} \quad \underset{r\to\infty}{\longrightarrow} \quad 0, d > 2 \implies \text{LRO} \tag{1.57}$$

$$\infty, d < 2 \implies \text{No LRO} \tag{1.58}$$

$$lnL \to \infty, d = 2 \implies \text{No LRO} \tag{1.59}$$

How do organisms beat this?

How motion beats Mermin-Wagner

How can motion make a difference? Now we will consider what will happen if we have movers and not pointers. We will look at frame of reference that is commoving with the flock. Suppose mean velocity of the flock is in upward direction. We will look at this blob of enhanced fluctuation as it grows. If it would have been pointer it would have grown by $distance \propto \sqrt{t}$ but inside this blob everyone is moving with wrong direction.

Whole blob is moving relative to the rest of the flock. Which direction is it moving? If the individual next to the one under consideration is not paying attention then it will try

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to keep pace with it. The component of speed in the direction of the individuals motion is almost same.

An individual can tell another individual outside of its neighbours if its moving with wrong speed by drifting to it and passing it by. Now, is this method of transport of information faster than the diffusion process. For this we need to compare the blob motion left and right with how big it grows as it diffuses. This we can get by simple power calculation. The typical lateral displacement roughly is $(RMS\ velocity) \times t$.

How far $\delta x_\perp$ does blob move $\perp \langle \vec{v} \rangle$?

$$\delta x_\perp \sim \sqrt{v_j^2 t} \sim v_0 \sqrt{\theta^2} t \tag{1.60}$$

Remember : $\sqrt{\theta^2} \propto r^{1-\frac{d}{2}} \propto t^{\frac{1}{2}-\frac{d}{4}}$

$$\Rightarrow \delta x_j \propto t^{\frac{3}{2}-\frac{d}{4}} \tag{1.61}$$

Compare with width of blob:

$$\frac{\delta x_\perp}{w(t)} \propto \frac{t^{\frac{3}{2}-\frac{d}{4}}}{t^{\frac{1}{2}}} \propto t^{1-\frac{d}{4}} \xrightarrow[t\to\infty]{} 0, d > 4 \tag{1.62}$$

$$\infty, d < 4 \tag{1.63}$$

Therefore, Bird motion dominates diffusion for $d < 4 \Rightarrow$ Physics changes in $d < 4$. "Breakdown of linearized hydrodynamics". So, what happens when $d < 4$?

To figure out the scaling laws. Self consistent calculation. Blob is defined as region that is affected by initially localized big fluctuation at the centre. The argument is the blob is going to grow anisotropically as shown in Fig.(1.7) i.e. diffusively as $\sqrt{t}$ in the direction of flock motion which we are taking in upward direction and laterally it grows at a greater pace $w_\perp(t)$. We will also estimate how big the errors are . The number of errors made per individual is proportional to time. And number of individual in the blob is proportional to the area of this region which in 2D is proportional to width times height which is $w_\perp(t)\sqrt{t}$ .We will do the same large number estimate and calculate the RMS value of error in the direction of motion is in this blob. Total number of error is $A(t)t$. RMS value be square root of this $A(t)t$. To find this for single individual we will divide by the area $A(t)$. This ratio will tell the typical angle of fluctuation inside the blob which goes as $\frac{t^{\frac{1}{4}}}{w_\perp^{\frac{1}{2}}}$.
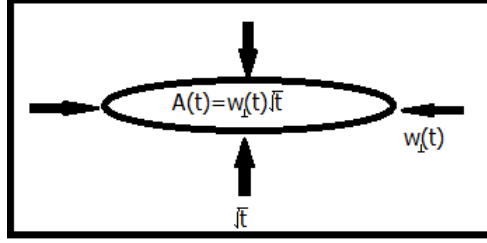
Figure 1.7: Anisotropic growth of the blob

$\Rightarrow$ Number of errors $\propto$ t

$\Rightarrow$ Number of spins $\propto$ A(t) $\propto w_\perp(t)\sqrt{t}$

$\Rightarrow$ Number of errors $\propto$ A(t)t $\propto w_\perp(t)t^{\frac{3}{2}}$

$\Rightarrow$ Number of errors/spin $\delta\theta \propto \dfrac{\sqrt{w_\perp(t)t^{\frac{3}{2}}}}{w_\perp(t)\sqrt{t}} \propto \dfrac{t^{\frac{1}{4}}}{w_\perp^{\frac{1}{2}}}$

We are considering a region which could be causally connected and the individual can affect each other in time t. And we are trying to estimate how big is the typical deviation of motion of the individual in this region from the flock as a whole is. And we are doing it similar to pointer case but the only difference is we know lateral motion is going to enhance transport in perpendicular direction which is different from $\sqrt{t}$. But we donot know how it increases. The information is transporting faster is because of the very fact that the birds are moving in wrong direction . By how much are they moving in wrong direction is

$$w_\perp(t) \sim v_0\delta\theta t \propto \frac{t^{\frac{5}{4}}}{w_\perp^{\frac{1}{2}}} \tag{1.64}$$

$$\Rightarrow \quad w_\perp^{\frac{3}{2}} \propto t^{\frac{5}{4}} \tag{1.65}$$

$$\Rightarrow \quad w_\perp \propto t^{\frac{5}{6}} >> t^{\frac{1}{2}} \tag{1.66}$$

And, so the typical distance of moving sideways is (typical lateral velocity)x(RMS error)x(time). So this angle $\delta\theta$ tells how much the blob is deviating from the direction of motion of the rest of the flock. Therefore, by this geometrical argument it is moving relatively fast laterally. In Mermin-Wagner argument $\delta\theta$ grew with time and that is why system ultimately disordered. Here $\delta\theta$ goes as $t^{-\frac{1}{6}}$. So as the blob grows it become closer to the mean direction of the flock. And so the system orders.

$$\delta\theta \propto \frac{t^{\frac{1}{4}}}{t^{\frac{5}{12}}} \propto t^{-\frac{1}{6}} \to 0 \tag{1.67}$$

as $t \to \infty \Rightarrow$ Long range Order

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Chapter 2

Isotropic-Nematic Transitions

There are examples of active matter where states with a uniaxial orientational order with $\hat{\mathbf{n}} \to -\hat{\mathbf{n}}$ symmetry ($\hat{\mathbf{n}}$ being the axis of orientation) have been observed. Such symmetries are observed in liquid crystals called nematics which are passive. However active nematics show significantly different behavior. In order to understand active nematics, I reviewed the physics of liquid crystals.

2.1   Liquid crystal physics

Liquid crystal are mesophases between crystalline solid and isotropic liquid.The are generally elongated or disklike. Their size is of few nanometer and the ratio between length : diameter or diameter : thickness of disk ≈ 5 or more. It possesses orientational order.[WY06, Hes15, And06]

At high temperature it exhibit isotropic phase with no positional and orientational order. If we reduce temperature it transforms to nematic phase which is a simplest liquid crystal phase wherein it has orientational order but no positional order. This means that, on the average, the long axis of the molecules of the liquid crystal point along a direction. This direction is denoted by $\hat{\mathbf{n}}$ which is a unit vector called liquid crystal director. This has $\hat{\mathbf{n}} \to -\hat{\mathbf{n}}$ symmetry. When temperature decreases further, it transforms to smectic phase which has orientational order and positional order only partially. This is because it arranges itself in layers. In a given layer, there is no poisitional order. With further reducing temperature, the form of this layered structure may change. At very low temperature, the material behaves like a crystal with both orientational and positional order.

2.1.1 Tensor Order Parameter

To understand the transitions we first characterize an order parameter. For the nematic, if $\mathbf{a}_i$ is a unit vector along the orientation of molecule i, the average of $\mathbf{a}_i$ is zero. Liquid crystals are centro-symmetric. Therefore, we cannot have a vector order parameter. The next higher order is a tensor. So we have to learn about tensors.

2.2 A tensor

A tensor of rank l is something with l indices, whose components in a rotated coordinate system are given as

$$A'_{\mu_1\mu_2...\mu_l} = U_{\mu_1\nu_1}U_{\mu_2\nu_2}....U_{\mu_l\nu_l}A_{\nu_1\nu_2....\nu_l}$$

2.2.1 Symmetric Second Rank Tensors

A symmetric second rank tensor is defined as $S_{\mu\nu} = S_{\nu\mu}$. It can be broken as Symmetric Second Rank Tensor = Isotropic + Symmetric Traceless part.

$$S_{\mu\nu} = \frac{1}{3}S_{\lambda\lambda}\delta_{\mu\nu}(isotropic) + S'_{\mu\nu}(\text{Symmetric-traceless}) \tag{2.1}$$

where

$$S'_{\mu\nu} = S_{\mu\nu} - \frac{1}{3}S_{\lambda\lambda}\delta_{\mu\nu} \tag{2.2}$$

This is invariant under a rotation of coordinate system. Since, $S'_{\nu\nu} = 0$, that is why this is symmetric traceless. It is generally referred to deviatoric part, because it tells about deviation from isotropy.[Hes15]

2.2.2 Principal Axes Representation

A symmetric tensor can be diagonalized by appropriate rotation of coordinate system. The corresponding axes in that coordinate system is called principal axes. In this system, it can be represented as

$$S := \begin{pmatrix} S^{(1)} & 0 & 0 \\ 0 & S^{(2)} & 0 \\ 0 & 0 & S^{(3)} \end{pmatrix}$$

with real eigen values $S_{(i)}, i = 1, 2, 3$. If unit vector that are parallel to these axes are $e^{(i)}, i = 1, 2, 3$, then ,

$$\mathsf{S} = \sum_{i=1}^{3} S^{(i)}e^{(i)}e^{(i)} \tag{2.3}$$

The eigen vectors are orthogonal $e^{(i)}.e^{(j)} = \delta^{(ij)}$ and complete $\sum_{i=1}^{3} e_\mu^{(i)}e_\nu^{(i)} = \delta_{\mu\nu}$. So, symmetric second rank tensor has 6 independent components in 3D.

Isotropic Tensors

$S^{(1)} = S^{(2)} = S^{(3)} = S$. Then **S** can be written as

$$S_{\mu\nu} = S\delta_{\mu\nu} \tag{2.4}$$

When 3 eigen values are unequal, the symmetric tensor has a non zero traceless part as we described before. Let us consider two cases: (i) two eigen values are equal and different from 3rd one. This is called unixial tensor (ii) All the three eigen values equal. This is called biaxial tensor.

Uniaxial tensor

$S^{(1)} = S^{(2)} \neq S^{(3)}$. Let, $S^{(1)} = S^{(2)} = S_\perp$, $S^{(3)} = S_\parallel$. Then,

$$S_{\mu\nu} = S_\parallel e_\mu e_\nu + S_\perp \left(\delta_{\mu\nu} - e_\mu e_\nu\right) \tag{2.5}$$

where $e = e^3$. We know,

$$e_\mu e_\nu = \frac{1}{3}\delta_{\mu\nu} + e'_\mu e'_\nu \tag{2.6}$$

So,

$$S_{\mu\nu} = S_\parallel \left[\frac{1}{3}\delta_{\mu\nu} + e'_\mu e'_\nu\right] + S_\perp \left(\delta_{\mu\nu} - \frac{1}{3}\delta_{\mu\nu}\right) \tag{2.7}$$

$$\Rightarrow S_{\mu\nu} = \frac{1}{3}\left(S_\parallel + 2S_\perp\right)\delta_{\mu\nu} + \left(S_\parallel - S_\perp\right)e'_\mu e'_\nu \tag{2.8}$$

In matrix notation, this becomes

$$\mathbf{S} = \frac{1}{3}\left(S_\parallel + 2S_\perp\right)\begin{pmatrix}1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1\end{pmatrix} + \left(S_\parallel - S_\perp\right)\begin{pmatrix}-\frac{1}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & \frac{2}{3}\end{pmatrix} \tag{2.9}$$

Biaxial Tensors

When $S^{(1)} \neq S^{(2)} \neq S^{(3)}$, the tensor is biaxial. We can write the tensor as,

$$S_{\mu\nu} = S''\delta_{\mu\nu} + se'^{(3)}_\mu e'^{(3)}_\nu + q\left(e'^{(1)}_\mu e'^{(1)}_\nu - e'^{(2)}_\mu e'^{(2)}_\nu\right) \tag{2.10}$$

where

$$S'' = \frac{1}{3}\left(S^{(1)} + S^{(2)} + S^{(3)}\right) \tag{2.11}$$

$$s = S^{(3)} - \frac{1}{2}\left(S^{(1)} + S^{(2)}\right) \tag{2.12}$$

$$q = \frac{1}{2}\left(S^{(1)} - S^{(2)}\right) \tag{2.13}$$

And $S^{(i)} = e_\mu^{(i)} S_{\mu\nu} e_\nu^{(i)}$,

$$e_\mu^{(i)} e_\mu'^{(j)} e_\nu'^{(j)} e_\nu^{(i)} = e^{(i)}\left[-\frac{1}{3}\delta_{\mu\nu} + e_\mu^{(j)} e^{(j)}\right] e_\nu^{(i)} \tag{2.14}$$

For $i = j$; $-\frac{1}{3} + 1 = \frac{2}{3}$. And for $i \neq j$; $-\frac{1}{3} + 0 = -\frac{1}{3}$. So,

$$S^{(1)} = S'' - \frac{1}{3}s + q \tag{2.15}$$

$$S^{(2)} = S'' - \frac{1}{3}s - q \tag{2.16}$$

$$S^{(3)} = S'' + \frac{2}{3}s \tag{2.17}$$

Using, $e_\mu'^{(1)} e_\nu'^{(1)} - e_\mu'^{(2)} e_\nu'^{(2)} = e_\mu^{(1)} e_\nu^{(1)} - e_\mu^{(2)} e_\nu^{(2)}$, $\mathbf{S} = \frac{1}{3}\sum_{i=1}^{3} S^{(i)} \delta_{\mu\nu} + \sum_{i=1}^{3} S^{(i)} e_\mu^{(i)} e_\nu^{(i)}$.
Now,

$$S^{(1)} e_\mu^{(1)} e_\nu^{(1)} + S^{(2)} e_\mu^{(2)} e_\nu^{(2)} =$$
$$\frac{1}{2}\left(S^{(1)} + S^{(2)}\right)\left(e_\mu'^{(1)} e_\nu'^{(1)} + e_\mu'^{(2)} e_\nu'^{(2)}\right)$$
$$+\frac{1}{2}\left(S^{(1)} - S^{(2)}\right)\left(e_\mu'^{(1)} e_\nu'^{(1)} - e_\mu'^{(2)} e_\nu'^{(2)}\right)$$

and $e_\mu'^{(1)} e_\nu'^{(1)} + e_\mu'^{(2)} e_\nu'^{(2)} = -e_\mu'^{(3)} e_\nu'^{(3)}$.
Using this we get to Eq. 2.10.

$$S_{\mu\nu} = S'' \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + s \begin{pmatrix} -\frac{1}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & \frac{2}{3} \end{pmatrix} + q \left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right]$$

$$S_{\mu\nu} = S'' \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \frac{2}{3}s \begin{pmatrix} -\frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} + q \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{2.18}$$

For a symmetric traceless tensor, $S^{(1)} + S^{(2)} + S^{(3)} = 0$ i.e. $S'' = 0$.
So, the anisotropic part is characterized by the linear combination of s and q of its principal values. For $q = 0, s \neq 0$, this is a uniaxial case Eq.(2.12) is recovered. When $s = 0, q \neq 0$

the symmetric traceless part of tensor is planar biaxial.

Scalar Invariants of a Symmetric Tensor

There are three quantities which are invariant under rotation of coordinate system called scalar invariant : (i) trace $I_1 = S_{\mu\mu}$ (ii) norm, $I_2 = S_{\mu\nu}S_{\mu\nu}$ (iii) determinant

$$I_3 = \det(\mathbf{S}) = \frac{1}{3}S_{\mu\nu}S_{\nu\lambda}S_{\lambda\mu} + \frac{1}{6}\left(S_{\mu\mu}S_{\nu\nu} - 3S_{\mu\nu}S_{\nu\mu}\right)S_{\lambda\lambda} \tag{2.19}$$

When rotated to the principal axes,

$$I_1 = S^{(1)} + S^{(2)} + S^{(3)} \tag{2.20}$$

$$I_2 = S^{(1)} + S^{(2)} + S^{(3)} \tag{2.21}$$

$$I_3 = S^{(1)}S^{(2)}S^{(3)} \tag{2.22}$$

For symmetric traceless tensors, $I_1 = 0$. Therefore,

$$I_2 = S'_{\mu\nu}S'_{\nu\mu}, \quad I_3 = 3\det(S') = S'_{\mu\nu}S'_{\nu\lambda}S'_{\lambda\mu} \tag{2.23}$$

This property will be used in calculating landau de Gennes free energy.

Biaxiality of a Symmetric Traceless Tensor

The principal values of a biaxial symmetric traceless tensor are $-\frac{1}{3}s + q$, $-\frac{1}{3}s - q$ and $\frac{2}{3}s$. Therefore, we obtain

$$I_2 = \frac{2}{3}s^2 + 2q^2, I_3 = 3det(S) = 2s\left(\frac{1}{9}s^2 - q^2\right) \tag{2.24}$$

We can define a biaxiality parameter b such that $b^2 = 1 - 6\frac{I_3^2}{I_2^3}$. So, $b^2 = 1$ for planar biaxial case and $b^2 = 0$ for uniaxial case since $I_3^2/I_2^2 = 1/6$.

2.2.3 Isotropic-Nematic Phase transition

Consider a single molecule of a nematic whose orientation is specified by a unit vector $\mathbf{u}$. The orientational distribution function is given by $f(\mathbf{u})$ and it is normalized, i.e. $\int f(\mathbf{u})d^2u = 1$. Also due to symmetry, $f(\mathbf{u}) = f(-\mathbf{u})$. This orientational distrbution function can be written down in terms of tensors of growing rank. The second rank tensor of that expansion is the smallest moment which can distinguish between isotropic and anisotropic distributions. This is given as

$$a_{\mu\nu} = \langle\phi_{\mu\nu}\rangle, \quad \phi_{\mu\nu} = \zeta_2 u'_\mu u'_\nu, \quad \zeta_2 = \sqrt{\frac{15}{2}} \tag{2.25}$$

Bracket resembles the average over orientational distribution. Note that $a_{\mu\nu}$ is a symmetric traceless tensor and in the coordinate representation of the principal axes, we can from our analysis of second rank symmetric traceless tensor conclude easily (using Eqs. 2.10-2.17) that,

$$a_{\mu\nu} = \sqrt{\frac{3}{2}} a_0 e'^{(3)}_\mu e'^{(3)}_\nu + \frac{1}{\sqrt{2}} a_1 \left(e^{(1)}_\mu e^{(1)}_\nu - e^{(2)}_\mu e^{(2)}_\nu \right). \tag{2.26}$$

Also $S'' = 0, s = \sqrt{\frac{3}{2}} a_0, q = \frac{a_1}{\sqrt{2}}$ and $I_2 = a_0^2 + a_1^2, I_3 = a_0(a_0^2 - 3a_1^2)$. With the choice $a_0 = a \cos\alpha$ and $a_1 = a \sin\alpha$, we get

$$I_2 = a^2, \quad I_3 = a^3 \cos 3\alpha, \quad b = \sin 3\alpha \tag{2.27}$$

where $b = \sqrt{1 - I_3^2/I_2^3}$ is the biaxiality parameter.

For nematics, $\alpha = 0, a_1 = 0$ and $a_0 = a$. Therefore,

$$a_{\mu\nu} = \sqrt{\frac{3}{2}} a e'^{(3)}_\mu e'^{(3)}_\nu = \sqrt{\frac{3}{2}} a n^{(3)}_\mu n^{(3)}_\nu$$

where $\mathbf{n} = e^{(3)}$ is the director. From here it follows that $a = \sqrt{5} S_2$ with $S_2 \equiv \langle P_2(\mathbf{u}.\mathbf{n}) \rangle$ where $P_2(x) = \frac{3}{2} \left(x^2 - \frac{1}{3} \right)$ is a second Legendre polynomial.

Landau-de Gennes Theory

To phenomenologically find out the isotropic-nematic phase transition, we describe the Landau-de Gennes potential in terms of the scalar invariants of the tensor order parameter $a_{\mu\nu}$ as

$$\phi \equiv \frac{1}{2} A I_2 - \frac{1}{3} B I_3 + \frac{1}{4} C I_2^2 \tag{2.28}$$

where $A = A_0 \left(1 - \frac{T*}{T} \right), A_0, B, C > 0$, where $T*$ is a temperature below the isotropic-nematic phase transition temperature. From the analysis above, we can express ϕ in terms of a and α

$$\phi^{LdG} = \frac{1}{2} A a^2 - \frac{1}{3} B a^3 \cos 3\alpha + \frac{1}{4} C a^4 \tag{2.29}$$

Now, the conditions for extremum

$$\frac{\partial\phi}{\partial\alpha} = B a^3 \sin 3\alpha = 0$$

and

$$\frac{\partial\phi}{\partial a} = aA - Ba^2 \cos 3\alpha + Ca^3 = 0$$

The first one implies that biaxility $b = \sin 3\alpha$ is zero. Therefore, the state is uniaxial with $\alpha = 0$. The second condition gives solutions $a = 0$ and $a = \frac{B}{2C} \pm \frac{1}{2C} \sqrt{B^2 - 4AC}$. The $a = 0$ is an isotropic state. In uniaxially ordered state $a \neq 0$. [And06]

Maier Saupe Theory

In the Maier Saupe theory, we write down the effective potential of single molecule with an orientation as

$$U_i(\theta_i) = -\frac{A}{V^2}S\left(\frac{3}{2}\cos^2(\theta_i) - \frac{1}{2}\right) \qquad (2.30)$$

where θ_i is angle between long axis of the molecule and director, V is volume of sample and A is constant independent of temperature

Knowing boltzmann probability,

$$P_i(\theta_i) = \frac{1}{Z}e^{-\frac{U_i(\theta_i)}{k_B T}} \qquad (2.31)$$

we get,

$$S = \langle \frac{3}{2}\cos\theta_i{}^2 - \frac{1}{2}\rangle = \int_0^\pi \left(\frac{3}{2}\cos^2\theta_i - \frac{1}{2}\right)P_i(\theta_i)\sin\theta_i d\theta_i \int_0^{2\pi} d\phi_i \qquad (2.32)$$

We know $P_i(\theta_i)$, therefore

$$S = \frac{1}{Z}\int_0^\pi \left(\frac{3}{2}\cos^2\theta_i - \frac{1}{2}\right)e^{-\frac{U_i(\theta_i)}{k_B T}}\sin\theta_i d\theta_i \int_0^{2\pi} d\phi_i \qquad (2.33)$$

So,

$$S = \frac{\int_0^\pi \frac{3}{2}\cos^2\theta_i e^{-\frac{U_i(\theta_i)}{k_B T}}sin\theta_i d\theta_i \int_0^{2\pi} d\phi_i - \frac{1}{2}\int_0^\pi e^{-\frac{U_i(\theta_i)}{k_B T}}sin\theta_i d\theta_i \int_0^{2\pi} d\phi_i}{\int_o^\pi e^{-\frac{U_i(\theta_i)}{k_B T}}sin\theta_i d\theta_i \int_0^{2\pi} d\phi_i}$$

$$S = \frac{\frac{3}{2}\int_0^\pi \cos^2\theta_i e^{-\frac{U_i(\theta_i)}{k_B T}}sin\theta_i d\theta_i}{\int_o^\pi e^{-\frac{U_i(\theta_i)}{k_B T}}sin\theta_i d\theta_i} - \frac{1}{2}$$

Now, $x = cos\theta_i \implies dx = -sin\theta_i d\theta_i$. Substituting,

$$S = \frac{\frac{3}{2}\int_1^{-1} -x^2 e^{-\frac{1}{k_B T}(-\frac{A}{V^2}S(\frac{3}{2}x^2 - \frac{1}{2}))}dx}{-\int_1^{-1} e^{-\frac{1}{k_B T}(-\frac{A}{V^2}S(\frac{3}{2}x^2 - \frac{1}{2}))}dx} - \frac{1}{2}$$

$$S = \frac{\frac{3}{2}\int_{-1}^1 x^2 e^{\frac{3ASx^2}{2k_B TV^2}}e^{-\frac{AS}{k_B TV^2}}dx}{\int_{-1}^1 e^{\frac{3ASx^2}{2k_B TV^2}}e^{-\frac{AS}{k_B TV^2}}dx} - \frac{1}{2}$$

Integral is an even function in x, so the integral from -1 to 1 becomes twice of 0 to 1. Now, let $m = \frac{3AS}{2k_B TV^2}$.

So,

$$S = \frac{\frac{3}{2}\int_0^1 x^2 e^{mx^2}dx}{\int_0^1 e^{mx^2}dx} - \frac{1}{2} \qquad (2.34)$$

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Now, let $mx^2 = t$.

So, $2mxdx = dt \implies xdx = \frac{dt}{2m}$,

$\int_0^1 x^2 e^{mx^2} dx = \frac{1}{2m} \int_0^m \sqrt{\frac{t}{m}} e^t dt = \frac{1}{2m\sqrt{m}} \int_0^m t^{1/2} e^t dt = \frac{1}{2m^{3/2}} \left[[t^{1/2} e^t]_0^m - \int_0^m \frac{1}{2\sqrt{t}} e^t dt \right]$

Substituting back we get,

$\int_0^1 x^2 e^{mx^2} dx = \frac{1}{2m^{3/2}} \left[\sqrt{m} e^m - \int_0^1 \frac{1}{\sqrt{m}} e^{mx^2} m dx \right] = \frac{e^m}{2m} - \frac{1}{2m} \int_0^1 e^{mx^2} dx$

So,

$$S = \frac{\frac{3}{2} \left[\frac{e^m}{2m} - \frac{1}{2m} \int_0^1 e^{mx^2} dx \right]}{\int_0^1 e^{mx^2} dx} - \frac{1}{2}$$

$$S = \frac{3}{4m} \left[\frac{e^m}{\int_0^1 e^{mx^2} dx} - 1 \right] - \frac{1}{2}$$

Now, let $y = \sqrt{m} x$, then,

$$S = \frac{3}{4m} \left[\frac{\sqrt{m} e^{y/x^2}}{\int_0^{\sqrt{m}} e^{y^2} dy} - 1 \right] - \frac{1}{2} \tag{2.35}$$

Now, we know $D(t) = e^{-t^2} \int_0^t e^{y^2} dy$, which is a Dawson's integral. If $t = y/x^2$, substitute in [2.77] to get,

$$S = \frac{3}{4m} \left[\frac{\sqrt{m}}{D(\sqrt{m})} - 1 \right] - \frac{1}{2} \tag{2.36}$$

Knowing m and S allows $(2k_B TV^2)/(3A)$, a quantity proportional to T, to be found from the definition of m. A graph of S versus T/T_{max}, where T_{max} corresponds to the largest value of $(2k_B TV^2)/(3A)$. The highest value of T occurs when S=0.32. Below T_{max} there are sometimes two values of S.

Now, the Helmholtz free energy is given by,

$$F = U - T\Sigma \tag{2.37}$$

where Σ is the entropy of the phase. The average energy of a molecule is:

$$\langle U_i \rangle = \langle -\frac{AS}{V^2} \left(\frac{3}{2} cos^2\theta - \frac{1}{2} \right) \rangle = \frac{AS}{V^2} \langle -\frac{3}{2} cos^2\theta - \frac{1}{2} \rangle = -\frac{AS^2}{V^2} \tag{2.38}$$

where $\langle ... \rangle$ denotes a thermal average using the probability $P_i(\theta_i)$ given before. Since this energy stems from an interaction between two molecules , to find the total energy for N molecules , we cannot simply multiply the average energy per molecule by N, since we would be counting the interaction energy of each pair of molecules twice. Therefore , the

total energy for N molecules is

$$U = -\frac{1}{2} N \frac{AS^2}{V^2} \tag{2.39}$$

The entropy of a single molecule is just,

$$\Sigma_i = -k_B \ln P_i(\theta_i) = \frac{U_i}{T} + k_B \ln Z \tag{2.40}$$

so the total Helmholtz free energy for N molecules is

$$F = -\frac{1}{2} \frac{NAS^2}{V^2} - \frac{NAS^2}{V^2} - Nk_BT \ln Z = N[\frac{1}{2} \frac{NAS^2}{V^2} - k_BT \ln Z] \tag{2.41}$$

Now, since $Z = 4\pi$ when we put S=0, so the free energy of isotropic phase is $-Mk_BTln(4\pi) = -2.53Nk_BT$. If the free energy of isotropic phase $\langle$ nematic phase , then nematic phase becomes unstable inspite of self consitent solution with non zero S exists. So as to have nematic phase to be stable it should have the value of its free energy smaller than this value. So to compute F for non zero S, Z should be expressed in terms of dawson's integral, to give

$$F = Nk_BT \left[\frac{mS}{3} - ln \left(\frac{4\pi}{\sqrt{m}} \exp \frac{2m}{3} D(\sqrt{m}) \right) \right] \tag{2.42}$$

Therefore, Maier Saupe theory predicts a first order transition at a temperature T_c defined by

$$k_BT_c = 0.22 \left[-\frac{N^2A}{V^2} \right] \tag{2.43}$$

Therefore, when value of S is below 0.43 , the isotropic phase has a lower free energy and therefore is a stable phase. Thus, the Maier Saupe theory predicts that the order parameter should decrease continuously from 0.43 to 0 at the transition to isotropic phase.

Chapter 3

Active Ising Model

In this chapter we will discuss about the 2D Active Ising Model and its simulation. For this we will start with defining 2D Ising model .

3.1   2D Ising Model

Ising model is defined for magnetic system where the system is made up of dipole moments placed within the material. It consistes of a lattice which for convenience we chose a square lattice suchg that there are magnetic dipole at each lattice site. Every site can accomodate a spin which can lie in two configurations i.e. ± 1 such that they represent upward or downward pointing spins. These spins will interact with nearest neighbours. For our purpose we will keep external magnetic field $B = 0$. The Hamiltonian will be of the form

$$H = -J \sum_{<ij>} s_i s_j - B \sum_i s_i \tag{3.1}$$

here the notation $< ij >$ denotes that the sites i and j are nearest neighbours. The minus sign here is conventional. The plot for energy can be seen in Fig.(3.1). Every state of Ising model consists of different values of spins. As we know each spin can take two such values so the number of states for lattice having N spins will be 2^N. So we ca write the partition function for the system as

$$Z = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} ... \sum_{s_N=\pm 1} = exp \left[\beta J \sum_{<ij>} s_i s_j + \beta B \sum_i s_i \right] \tag{3.2}$$

In shorter notation,

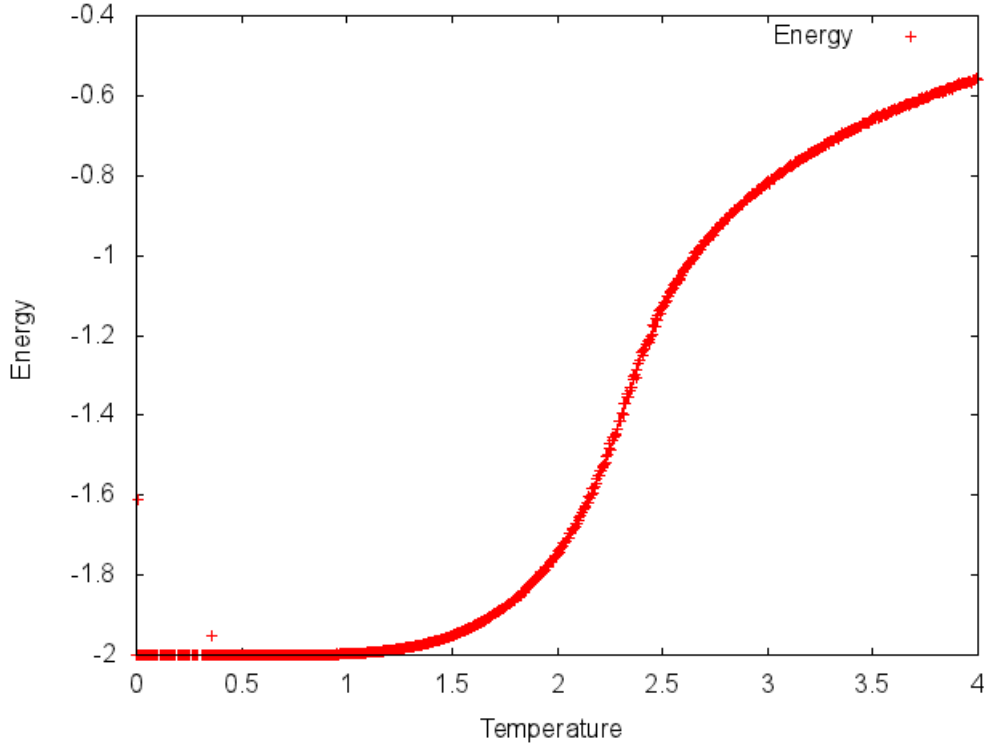$$Z = \sum_{s_i} e^{-\beta H} \tag{3.3}$$

Figure 3.1: The energy is continuous function of temperature.

We can also calculate the mean magnetization $\langle M \rangle$ of the model from the partition function using ,

$$M = \frac{\partial(-kTlogZ)}{\partial B} \tag{3.4}$$

although as we will see it is usually simpler to evaluate $\langle M \rangle$ directly from an average over states :

$$\langle M \rangle = \langle \sum_i s_i \rangle \tag{3.5}$$

Often, in fact, we are more interested in the mean magnetization per spin $\langle m \rangle$ which can be seen in Fig.(3.2), which is just

$$\langle m \rangle = \frac{1}{N} \langle \sum_i s_i \rangle \tag{3.6}$$

We can calculate fluctuations in the magnetization or the internal energy by calculating derivatives of the partition function. We can calculate the magnetic susceptibility per spin:

$$\chi = \frac{\beta}{N}(\langle M^2 \rangle - \langle M \rangle^2) = \beta N(\langle m^2 \rangle - \langle m \rangle^2) \tag{3.7}$$
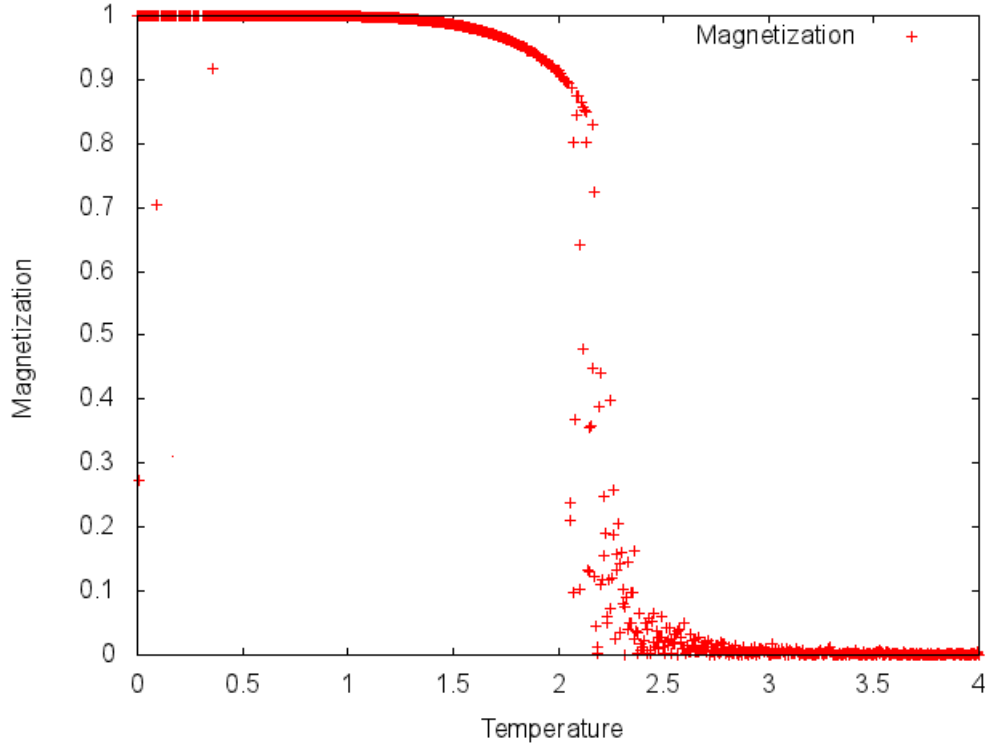
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Figure 3.2: Fall in magnetization around critical temperature~ 2.3

The graph for this can be seen in Fig.(3.4). Similarly we can calculate the specific heat per spin c from the energy fluctuations thus:

$$c = \frac{k\beta^2}{N} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \tag{3.8}$$

This has been plotted in Fig. 3.3. The simulations were done on a two dimensional lattice using Monte Carlo technique [NB99].

3.2 2D Active Ising Model

Active systems are large collection of interacting particles which consume energy to self-propel and are known to show elaborate collective behaviour. A coherent displacement can be seen over length scales a lot larger than individual size. This can be observed in a diverse biological system like fish schools, bacterial swarm , bird flocks, microtubule motility assays and even in inert matter which is artificially self propelled. This collective motion transitioning to flocking has aroused interest in many physicist.

The Vicsek model has been prototypical for this area of research with two properties namely self propulsion at constant speed and alignment with neighbours. It has been
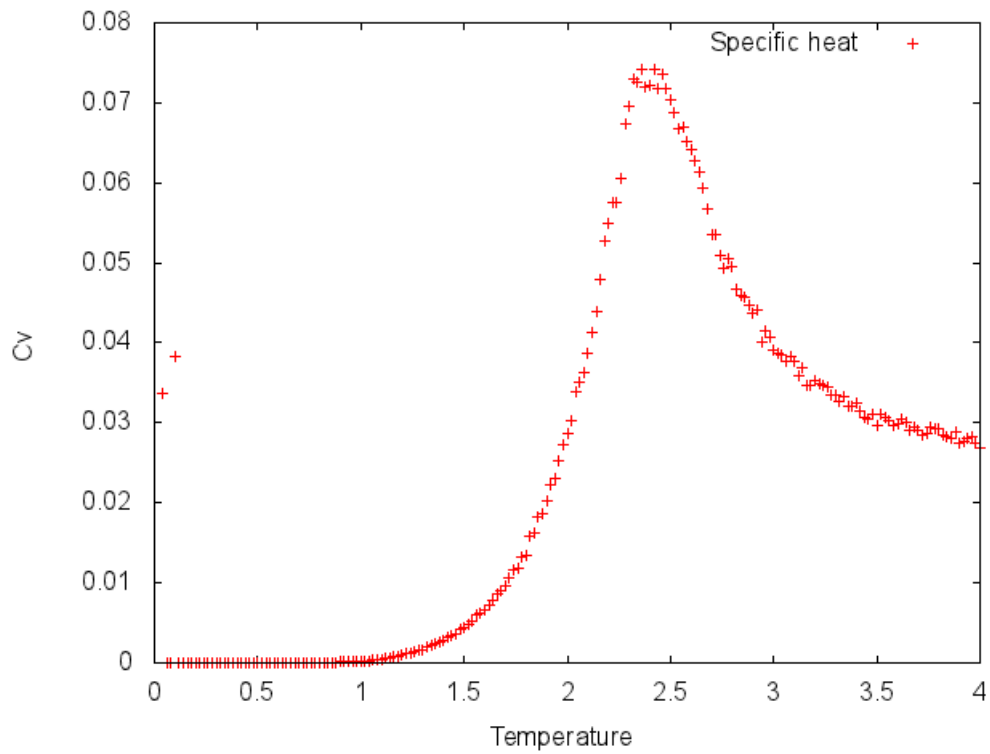
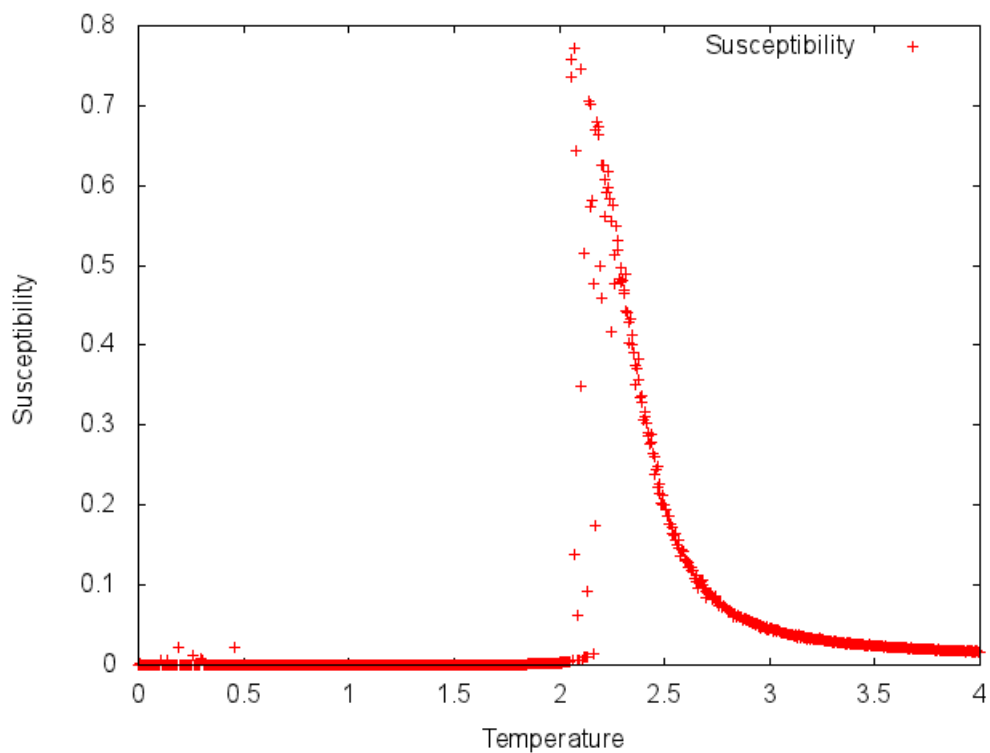Figure 3.3: Peak in specific heat at critical temperature

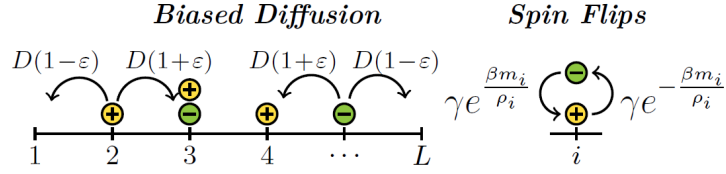Figure 3.4: Susceptibility shows a jump at critical temperature

Figure 3.5: Sketch of the possible actions and their rates of occurence

described using X-Y Model. On reducing the noise in the aligning interaction or else increasing density , a transition is observed from disordered gas phase to an ordered collective motion. Amidst these homogeneous phase lies a region of parameter space where these individual particles gather in ordered bands in between dilute disordered background. Such bands are frequently observed in flocking models and resembles 1st order phase transition. This is seen only in large systems.

Because of the scale of the problem , the analytical approaches have been deviced. Hydrodynamic equations have been tried to derive either phenomenonologically or by coarse graining.Such equation facilitate in predicting phase transition which is in qualitative agreement to microscopic model along with emergence of inhomogeneous bands. Inspite of the usefulness of the analutical approach, the equation which are dealt with are linearized because of the complications. But we can see long range order nevertheless.

Complete analytical study of Vicsek Model is extremely complicated so we will deal with this problem through an alternative strategy by introducing Active Ising Model(AIM). The use of non-equilibrium version of ferromagnetic model has been fruitful. The form of AIM in consideration exhibit two kinds of properties : 1) Self propulsion 2) Aligning interaction. The continuous rotational symmetry in Vicsek model is replaced by discrete symmetry. The particles here are diffusive in nature but propelled in one direction. AIM makes the understanding simpler in addition to retaining most of the properties. Lattice based model simplify both analytical and numerical study.

3.2.1 Definition of Model:

Consider N particles which are on a two dimensional lattice. The total number of sites in the lattice is $L_x \times L_y$. Every particle is assigned a spin variable $s = \pm 1$. Unlike the Ising model, here any number of particles can occupy a given site. To every site we can assign a local density $\rho_i = n_i^+ + n_i^-$ and a local magnetization $m_i = n_i^+ - n_i^-$. $n_i^\pm$ are the number of particles with spin ± 1 on lattice site i. The evolution happens by spins flipping on a
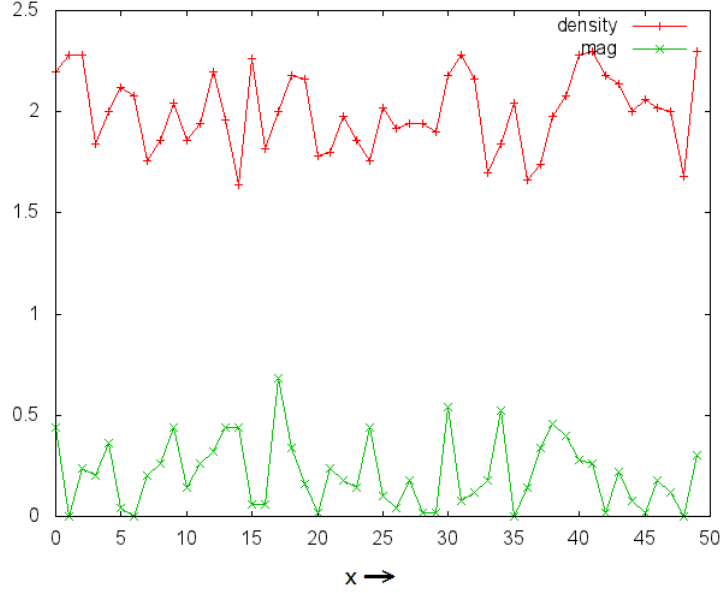
Figure 3.6: Density profiles (red upper line) and magnetization profiles (green lower line) averaged along vertical direction showing the disordered gas phase. Here $\beta = 1.4$, $\rho_o = 2$, $D = 1$ and $\varepsilon = 0.9$.

lattice site (like the Ising model) as well as hopping from one lattice site to another (unlike Ising model) [ST13, ST15].

A spin on a lattice site flips according to

$$W(s \rightarrow -s) = \gamma exp\left(-s\beta\frac{m_i}{\rho_i}\right) \tag{3.9}$$

with $\beta = 1/T$. This is a local interaction since particles on a lattice site will only allign with other particles which occupy the same site. This move therefore causes alignment.

3.2.2   Self-propulsion:

A particle on a lattice site can also hop to other particles in neighbouring sites. On a 2d square lattice, it hops to the right with rate $D(1 + s\varepsilon)$ and to the left with rate $D(1 - s\varepsilon)$. This difference in rates ensures that the particles move in a definite direction therefore giving the self propulsion mechanism. The propulsion is tuned with the parameter ε. D is the normal diffusion rate. Therefore, when $\varepsilon \rightarrow 0$, the spins will just diffuse. Note that hopping to the top and bottom is with rate D.

Figure 3.7: Density profiles (red upper line) and magnetization profiles (green lower line) averaged along vertical direction showing the polar liquid phase. Here, $\beta = 2$, $\rho_0 = 7$, $D = 1$ and $\varepsilon = 0.9$.
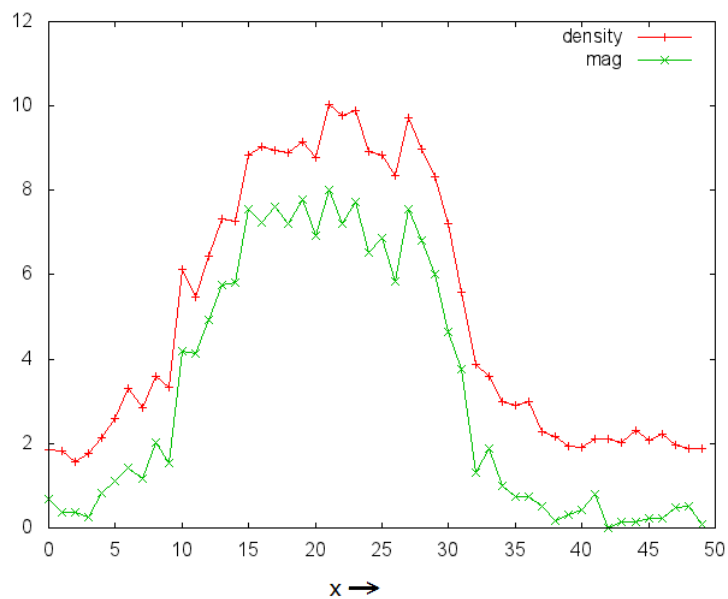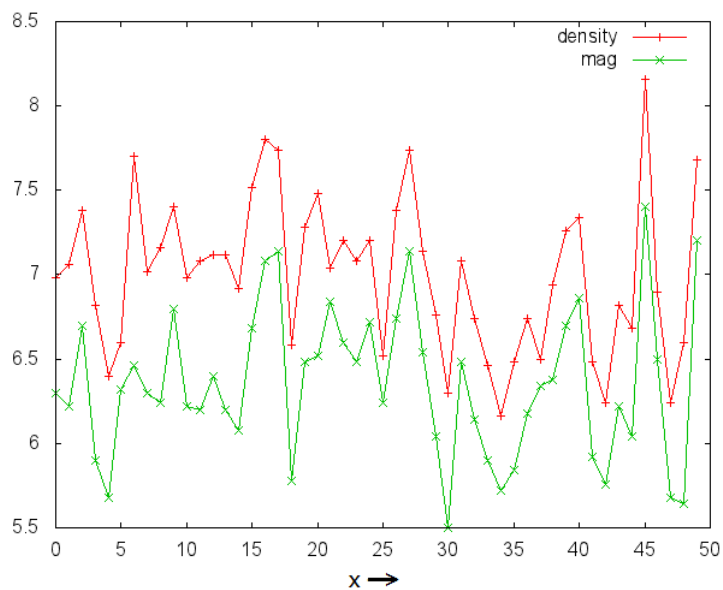

Figure 3.8: Density profiles (red upper line) and magnetization profiles (green lower line) averaged along vertical direction for the liquid-gas coexistence phase. Here, $\beta = 1.6$, $\rho_0 = 5$, $D = 1$ and $\varepsilon = 0.9$.
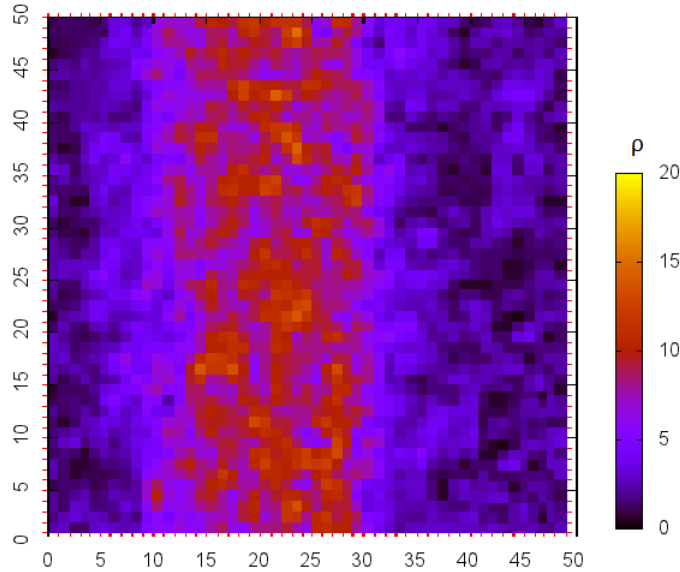
Figure 3.9: 2d snapshot of a 50×50 lattice corresponding to liquid-gas coexistence.

3.2.3   Simulations

The simulations were carried out using random-sequential update. In a time Δt, a randomly chosen particle is flipped with a probability given as $W(s \to -s)\Delta t$, hops downwards and upwards with probabilities $D\Delta t$, to left and right with probabilities $D(1 \mp s\varepsilon)\Delta t$. Lastly, the probability of doing nothing will be $1 - [4D + W(s \to -s)]\Delta t$.

3.2.4   Liquid-Gas Phase Transition

In my project I simulated the active Ising model and observed three different phases in the parameter space of the temperature $T = \beta^{-1}$, the average density $\rho_0 = \frac{N}{LxLy}$, and ε (Figs. 3.6, 3.7, 3.8). When the temparature is high and the density is low, the particles are randomy oriented and do not self organize. Therefore, we get a homogeneous gaseous phase . However, for large densities and small temperatures, we see particles moving together either to left or right. At densities in between these densities, the system phase seperates and a band of polar particles travel to the left or right in a background of particles randomly oriented.

Appendix A

C++ Code for 2D Ising Model

```cpp
#include <fstream>
#include <stdio.h>
#include <conio.h>
#include <math.h>
#include <time.h>
#include <stdlib.h>
#include <iostream>
using namespace std;
int main()
{
 int Nx,Ny;
scanf("%d %d",&Nx,&Ny);
freopen("ans.txt","w",stdout);
int S[Nx][Ny]; double E1=0.0,E2=0.0,dE=0.0,r,temp1,t,AvgE=0.0,
AvgEf=0.0,AvgMf=0.0,M2=0.0,AvgM2=0.0,Sus=0.0,Heat=0.0,E3=0.0,
AvgE3=0.0;
int N=Nx*Ny;
double M1=0,AvgM=0;
double M[200];
double E[200];
double T[200];
int z=0,i,j,m,n;
int i1=i+1;
int i2=i-1;
int j1=j+1;
int j2=j-1;
```

```c
int m1=m+1;
int m2=m-1;
int n1=n+1;
int n2=n-1;
for(t=4.0;t>=0.02;t=t-0.02)
   {
        for(i=0;i<Nx;i=i+1)
          {
          for(j=0;j<Ny;j=j+1)
            {
                if((double)rand()/RAND_MAX < 0.5)
                   S[i][j]=1;
                else
                   S[i][j]=-1;
            }
          }
E1=0.0;
E2=0.0;
dE=0.0;
double r=0.0;
temp1=0.0;
AvgE=0.0;
AvgEf=0.0;
M1=0;
AvgM=0;
AvgMf=0.0;
AvgM2=0.0;
AvgE3=0.0;
M2=0.0;
Sus=0.0;
Heat=0.0;
E3=0.0;
for(i=0;i<Nx;i=i+1)
{
for(j=0;j<Ny;j=j+1)
    {
        i1=i+1;
        i2=i-1;
        j1=j+1;
```

```
  j2=j-1;
 if(i==(Nx-1))
     i1=0;
 if(i==0)
     i2=Nx-1;
 if(j==(Ny-1))
     j1=0;
 if(j==0)
     j2=Ny-1;
 E1=E1-S[i][j]*(S[i1][j]+S[i][j1]+S[i2][j]+S[i][j2])/2;
 }
}
   for(int k=1;k<=10000;k=k+1)
    {
   for(int x=0;x<Nx;x=x+1)
       {
      for(int y=0;y<Ny;y=y+1)
          {
             E2=0.0;
           S[x][y]=-S[x][y];
             for(m=0;m<Nx;m=m+1)
          {
                for(n=0;n<Ny;n=n+1)
                 {
                  m1=m+1;
                  m2=m-1;
                  n1=n+1;
                  n2=n-1;
                  if(m==(Nx-1))
                     m1=0;
                  if(m==0)
                     m2=Nx-1;
                  if(n==(Ny-1))
                     n1=0;
                  if(n==0)
                     n2=Ny-1;
                  E2=E2-S[m][n]*(S[m1][n]+S[m][n1]+S[m2][n]+S[m][n2])/2;
                 }
              }
```

```
            dE=E2-E1;
            if(dE<=0)
                E1=E2;
            else
             {
                r=(double)rand()/RAND_MAX;
                temp1=(double) exp(-dE/t);
                if(r<temp1)
                    E1=E2;
                else
                    S[x][y]=-S[x][y];
             }
         }
     }
}
E1=0.0;
E2=0.0;
dE=0.0;
r=0.0;
temp1=0.0;
AvgE=0.0;
M1=0;
AvgM=0;
M2=0.0;
E3=0.0;
for(i=0;i<Nx;i=i+1)
{
    for(j=0;j<Ny;j=j+1)
     {
        i1=i+1;
        i2=i-1;
        j1=j+1;
        j2=j-1;
        if(i==(Nx-1))
            i1=0;
        if(i==0)
            i2=Nx-1;
        if(j==(Ny-1))
            j1=0;
```

```
          if(j==0)
              j2=Ny-1;
          E1=E1-S[i][j]*(S[i1][j]+S[i][j1]+S[i2][j]+S[i][j2])/2;
          M1=M1+S[i][j];
      }
}
 for(int k=0;k<10000;k=k+1)
 {
      for(int x=0;x<Nx;x=x+1)
        {
            for(int y=0;y<Ny;y=y+1)
             {
                E2=0.0;
                S[x][y]=-S[x][y];
                for(m=0;m<Nx;m=m+1)
                  {
                      for(n=0;n<Ny;n=n+1)
                        {
                        m1=m+1;
                        m2=m-1;
                        n1=n+1;
                        n2=n-1;
                        if(m==(Nx-1))
                            m1=0;
                        if(m==0)
                            m2=Nx-1;
                        if(n==(Ny-1))
                            n1=0;
                        if(n==0)
                            n2=Ny-1;
                        E2=E2-S[m][n]*(S[m1][n]+S[m][n1]+S[m2][n]+S[m][n2])/2;
                        }
                  }
            dE=E2-E1;
            if(dE<=0)
            {
                E1=E2;
                M1=M1+2*S[x][y];
            }
```

```
                else
                {
                    r=(double)rand()/RAND_MAX;
                    temp1=(double) exp(-dE/t);
                    if(r<temp1)
                     {
                        E1=E2;
                        M1=M1+2*S[x][y];
                     }
                     else
                         S[x][y]=-S[x][y];
                }}}
        AvgE=AvgE+(E1/N);
        AvgM=AvgM+(M1/N);
        M2=M2+ (M1/N)*(M1/N);
        E3=E3+ (E1/N)*(E1/N);
     }
    AvgEf=AvgE/10000;
    AvgMf=AvgM/10000;
    AvgM2=M2/10000;
    AvgE3=E3/10000;
    Sus=AvgM2-AvgMf*AvgMf;
    Heat=AvgE3-AvgEf*AvgEf;
    E[z]=AvgEf;
    if(AvgMf<0)
        AvgMf=-AvgMf;
    M[z]=AvgMf;
    T[z]=t;
    cout << T[z]<<"\t \t"<<M[z]<<"\t \t"<<E[z]<<"\t \t"<<Sus<<"\t \t"<<Heat<<"\n";
    z=z+1;
 }
 for(int g=0;g<Nx;g++)
   {
      for(int h=0;h<Ny;h++)
       {
       cout<<g<<"\t \t"<<h<<"\t \t"<<S[g][h]<<"\n";
     } } }
 return 0;
}
```

Appendix B

C++ Code for 2D Active Ising Model

```cpp
#include <fstream>
#include <stdio.h>
#include <cmath>
#include <math.h>
#include <time.h>
#include <stdlib.h>
#include <iostream>
using namespace std;
int main()
{
int Nx,Ny;
double EPSILON =0.0000001;
double sum=0.0,sum1=0.0;
int q;
scanf("%d %d",&Nx,&Ny);
freopen("ans.txt","w",stdout);
int N=Nx*Ny;//no of lattice sites
double S[N][4];//lattice details(n+,n-,rho,m)
int rho0=7;//initial density
int N1=rho0*N;//no of particles
int B[N1][2];//spin location and configuration(lattice site,spin)
int randNum=0;
int min=0,max=N1-1,max1=N-1;
int D=1;
double e=0.9;
```

```
double b,E1=0.0,W=0.0,dt=0.0;
int neigh[4];//right,left,up,down
for(int i=0;i<N;i++)//initialized 0 to the array
{
S[i][0]=0;
S[i][1]=0;
S[i][2]=0;
S[i][3]=0;
}
for(int i=0;i<N1;i++)//initialized 0 to the array
{
B[i][0]=0;
B[i][1]=0;
}

for(int i=0;i<N1;i=i+1)//randomly distributed the particles over the lattice
{
int r=rand()%(max1-min+1)+min;//generated random no between 0 to(N-1) to place the particles
if((double)rand()/RAND_MAX < 0.5)//randomly selecting a +1/-1 configuration and updating tha
{
S[r][0]=S[r][0]+1;//no of +1 spin is in 1st column
B[i][1]=1;
}
else
{
S[r][1]=S[r][1]+1;//no of -1 spin is in 2nd column
//S[r][0]=S[r][0]+0;
B[i][1]=-1;
}
S[r][2]=S[r][0]+S[r][1];
S[r][3]=S[r][0]-S[r][1];
B[i][0]=r;
}

  for(b=2.5;b>=0.0;b=b-0.1)//using this instead of t
 {
b=2;
dt=1/(4*D+exp(b));//already defined
 E1=0.0;
```

```
for(int i=0;i<N;i++)
{
  E1=E1-S[i][3]*S[i][3]/(2*S[i][2]);
}
 printf("%f \n",b);
for(int k=1;k<=10000;k=k+1)//montecarlo steps
{
for(int x=0;x<N1;x=x+1)
{
int randNum = rand()%(max-min + 1) + min;//integer random generator bet 0 to (N1-1)
//so we selected a particle and now we will use its location to find the neighbours
int h=B[randNum][0];
 printf("before");
 printf("%d %f %f %f %f \n",h,S[h][0],S[h][1],S[h][2],S[h][3]);
if((h+1)%Ny==0)  //right point
neigh[0]=h-Ny+1;
else
neigh[0]=h+1;

if(h%Ny==0)  //left point
neigh[1]=h+Ny-1;
else
neigh[1]=h-1;

if(h<Ny)   //upper point
neigh[2]=h+(Nx-1)*Ny;
else
neigh[2]=h-Ny;

if((h+Ny)>=(Nx*Ny))//lower point
neigh[3]=h-(Nx-1)*Ny;
else
neigh[3]=h+Ny;

    printf("%d %f %f %f %f \n",neigh[0],S[neigh[0]][0],S[neigh[0]][1],
    S[neigh[0]][2],S[neigh[0]][3]);
    printf("%d %f %f %f %f \n",neigh[1],S[neigh[1]][0],S[neigh[1]][1],
    S[neigh[1]][2],S[neigh[1]][3]);
    printf("%d %f %f %f %f \n",neigh[2],S[neigh[2]][0],S[neigh[2]][1],
```

```c
    S[neigh[2]][2],S[neigh[2]][3]);
    printf("%d %f %f %f %f \n",neigh[3],S[neigh[3]][0],S[neigh[3]][1],
    S[neigh[3]][2],S[neigh[3]][3]);
W=exp(-B[randNum][1]*S[h][3]*b/(S[h][2]));//condition to flip
if((double)rand()/RAND_MAX <= W*dt)//flipping
{
    printf("flipping");
if(B[randNum][1]==1)
{
S[h][0]=S[h][0]-1;
S[h][1]=S[h][1]+1;
S[h][3]=S[h][3]-2;
B[randNum][1]=-1;
}
else if(B[randNum][1]==-1)
{
S[h][0]=S[h][0]+1;
S[h][1]=S[h][1]-1;
S[h][3]=S[h][3]+2;
B[randNum][1]=1;
}
}
break;
if(W*dt<(double)rand()/RAND_MAX<=W*dt+D*(1+B[randNum][1]*e)*dt)//hopping to the right
{
    printf("hop right");
if(B[randNum][1]==1)
{
S[h][0]=S[h][0]-1;
S[neigh[0]][0]=S[neigh[0]][0]+1;
S[h][2]=S[h][2]-1;
S[neigh[0]][2]=S[neigh[0]][2]+1;
S[h][3]=S[h][3]-1;
S[neigh[0]][3]=S[neigh[0]][3]+1;
B[randNum][0]=neigh[0];
}
else if(B[randNum][1]==-1)
{
S[h][1]=S[h][1]-1;
```

```c
S[neigh[0]][1]=S[neigh[0]][1]+1;
S[h][2]=S[h][2]-1;
S[neigh[0]][2]=S[neigh[0]][2]+1;
S[h][3]=S[h][3]+1;
S[neigh[0]][3]=S[neigh[0]][3]-1;
B[randNum][0]=neigh[0];
}
}
break;
if(W*dt+D*(1+B[randNum][1]*e)*dt<(double)rand()/RAND_MAX<=W*dt+2*D*dt)//hopping to the
                                                                  left
{
 printf("hop left");
if(B[randNum][1]==1)
{
S[h][0]=S[h][0]-1;
S[neigh[1]][0]=S[neigh[1]][0]+1;
S[h][2]=S[h][2]-1;
S[neigh[1]][2]=S[neigh[1]][2]+1;
S[h][3]=S[h][3]-1;
S[neigh[1]][3]=S[neigh[1]][3]+1;
B[randNum][0]=neigh[1];
}
else if(B[randNum][1]==-1)
{
S[h][1]=S[h][1]-1;
S[neigh[1]][1]=S[neigh[1]][1]+1;
S[h][2]=S[h][2]-1;
S[neigh[1]][2]=S[neigh[1]][2]+1;
S[h][3]=S[h][3]+1;
S[neigh[1]][3]=S[neigh[1]][3]-1;
B[randNum][0]=neigh[1];
}
}
break;
if(W*dt+2*D*dt<(double)rand()/RAND_MAX<=W*dt+3*D*dt)hopping up
{

    printf("hop up");
```

```c
if(B[randNum][1]==1)
{
S[h][0]=S[h][0]-1;
S[neigh[2]][0]=S[neigh[2]][0]+1;
S[h][2]=S[h][2]-1;
S[neigh[2]][2]=S[neigh[2]][2]+1;
S[h][3]=S[h][3]-1;
S[neigh[2]][3]=S[neigh[2]][3]+1;
B[randNum][0]=neigh[2];
}
else if(B[randNum][1]==-1)
{
S[h][1]=S[h][1]-1;
S[neigh[2]][1]=S[neigh[2]][1]+1;
S[h][2]=S[h][2]-1;
S[neigh[2]][2]=S[neigh[2]][2]+1;
S[h][3]=S[h][3]+1;
S[neigh[2]][3]=S[neigh[2]][3]-1;
B[randNum][0]=neigh[2];
}
}
break;
if(W*dt+3*D*dt<(double)rand()/RAND_MAX<=W*dt+4*D*dt)hopping down
{
 printf("hop down");
if(B[randNum][1]==1)
{
S[h][0]=S[h][0]-1;
S[neigh[3]][0]=S[neigh[3]][0]+1;
S[h][2]=S[h][2]-1;
S[neigh[3]][2]=S[neigh[3]][2]+1;
S[h][3]=S[h][3]-1;
S[neigh[3]][3]=S[neigh[3]][3]+1;
B[randNum][0]=neigh[3];
}
else if(B[randNum][1]==-1)
{
S[h][1]=S[h][1]-1;
S[neigh[3]][1]=S[neigh[3]][1]+1;
```

```
S[h][2]=S[h][2]-1;
S[neigh[3]][2]=S[neigh[3]][2]+1;
S[h][3]=S[h][3]+1;
S[neigh[3]][3]=S[neigh[3]][3]-1;
B[randNum][0]=neigh[3];
}
}


  printf("after");
  printf("%d %f %f %f %f \n",h,S[h][0],S[h][1],S[h][2],S[h][3]);
   printf("%d %f %f %f %f \n",neigh[0],S[neigh[0]][0],S[neigh[0]][1],S[neigh[0]][2],
   S[neigh[0]][3]);
  printf("%d %f %f %f %f \n",neigh[1],S[neigh[1]][0],S[neigh[1]][1],S[neigh[1]][2],
  S[neigh[1]][3]);
    printf("%d %f %f %f %f \n",neigh[2],S[neigh[2]][0],S[neigh[2]][1],S[neigh[2]][2],
    S[neigh[2]][3]);
 printf("%d %f %f %f %f \n",neigh[3],S[neigh[3]][0],S[neigh[3]][1],S[neigh[3]][2],
 S[neigh[3]][3]);


}
}
  printf("%f \n", b);
      if(b==1.600000)//i want to plot for this value
     if(fabs(b - 1.6) < EPSILON)//to print only b=1.6
   {
 printf("-----------------------sI am happy");
for(int f=0;f<N;f=f+1)
{
 printf("%d %d \n",f,S[f][2]);
 }
 int p=0;
 for(int i=0;i<Nx;i++)//to print in the form of square lattice
 {
      for(int j=0;j<Ny;j++)
       {
            printf("%d %d %f \n",i,j,S[p][2]);
            p=p+1;
            }
            printf("\n");
```

```
    }
 for(int z=0;z<N;z++)
 {
   printf("%d %f %f %f %f \n",z,S[z][0],S[z][1],S[z][2],S[z][3]);
  }
for(int i=0;i<Ny;i++)
{   sum=0.0;
sum1=0.0;
q=i;
for(int j=0;j<Nx;j++)
{
sum1=sum1+S[q][3];
sum=sum+S[q][2];
q=q+Ny;
}
sum1=sum1/Nx;
sum=sum/Nx;
printf("%d %f %f \n",i,sum, sum1);
}
}
  }
}
```

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