Chapter 1

Introduction

Abbreviations/Acronyms: **ABP** (active Brownian particle), **ABPs** (active Brownian particles), **AMB** (active model B), **AMBN** (active model B with noise), **CHC** (Cahn-Hilliard-Cook), ***FDT***(fluctuation-dissipation theorem), **HCP** (hexagonal close packed), **MIPS** (motility induced phase separation), **SPP** (self propelled particle), **SPPs** (self propelled particles), **TDGL** (time-dependent Ginzburg Landau).

1.1 Statistical mechanics:macro to micro

Statistical mechanics gives us tools to achieve the goal of understanding the relationship between microscopic and macroscopic properties of the system and provides a bridge between them. In place of using the detail of each constituent particle of a macroscopic system, it helps us in finding a qualitative way to design a microscopic model and explain the origin of the behavior observed in equilibrium and nonequilibrium systems. The equilibrium system in statistical mechanics is described by probability distributions of microstates where the distribution function does not change with time. On the other hand, the probability distribution of microscopic states of a nonequilibrium system changes with time so they are characterised by time dependent distribution functions. Foundation of statistical mechanics started from the major contribution of Ludwig Boltzmann L.Boltzmann (1964); Uffink (2004) whose methods have been applied to wide range of physical systems. The works of other scientists like James Clerk Maxwell Grant & Phillips (2013), Josiah Willard Gibbs Klein (1990), and Albert Einstein Sen (2021) played a remarkable role in formulating it. It grew from the thermodynamics as the thermodynamic properties were needed a more detailed formulation in terms of dealing with deeper degrees of freedom and analysing the underlying microscopic behavior K.Huang (2008); Pathria (1996); Paul M (1995); Zemansky & Dittman (1997). The key idea of statistical mechanics involves the averaging of any statistical quantity over the system details and calculating the statistical fluctuations for different length and time scales.

1.2 Ensembles, phase space and thermodynamic averages

To understand the link between statistical mechanics and thermodynamics, it's needed to introduce the thermodynamic ensemble, which are classified on the basis of fixed value of number of particles, N, total energy E, volume, V temperature T and chemical potential μ in their respective ensembles Pathria (1996); Paul M (1995); Zemansky & Dittman (1997). The most commonly used are :*Microcanonical (N, E, V), Canonical (T, V, N), and Grand canonical ensemble (T, V,*μ*).* Along with these three ensembles there are other ones also relevant in different contexts like Isobaric-Isenthalpic (N,P,H),Isothermal-Isobaric (N,P,T),Gibbs ensemble (N,P,T,μ) and Gibbs-Helmholtz ensemble (N,V,T,μ). There are other ensembles also where external factors , such as electric fields, surface tension, or mechanical deformations plays an important role that is not relevant to discuss here. The macrostate of a physical system of N number of identical particles confined in a space of volume V and total energy E is defined by variables (N, V, E). Now, since the total energy E of the system can be distributed among N particles in various possible ways which defines the various possible arrangements and these arrangements refer to the microstate of the system. Therefore a system of N number of particles in $3-dimensional$ space requires $6N$ degrees of freedom to describe it completely where $3N$ is for position coordinates and $3N$ is for momentum coordinates. This $6N$ dimensional space is known as phase space and each point in phase space denotes a microstate of the system Bhattacharyajee (2000); Pathria (1996); Zemansky & Dittman (1997). A given macrostate consists a number of microstates. In the microscopic approach, in place of keeping track of each degrees of freedom, we use statistical description to define the probability dP of the system in an elemental volume dV of the phase space. The probability dP is defined as $dP = lim_{t\to\infty}\frac{dt}{T}$, where dt represent the time spent by the system in the volume element dV and T is the total time over which system is tracked. One can do the averaging of any statistical quantity using the approach of time averaging or ensemble averaging. Time average of any statistical quantity,$f(t)$ along a trajectory is defined by $\overline{f} = lim_{\tau\to\infty}\frac{1}{\tau}\int_0^{\tau} f(t)dt$ Pathria (1996); Zemansky & Dittman (1997). Approach of ensemble averaging treats each phase point in the phase space as different copies of the same system called an ensemble. Let $\overline{N}$ is the number of copies corresponds to the volume V, and $\overline{dN}$ is the number of copies corresponding to volume element dV, then the probability of the system being in volume V is defined as $d\overline{P} = lim_{\overline{N}\to\infty}\frac{d\overline{N}}{\overline{N}} = \rho(q_i, p_i)dV$, where q_i, p_i, and $\rho(q_i, p_i)$ are $3N$ position, momentum coordinates, and density in the phase space respectively. Average of any quantity f can be calculated by defining $\overline{f} = \int f\rho dV$, where ρ is the probability density function Pathria (1996); Zemansky & Dittman (1997). Now, it becomes important to discuss the three postulates of equilibrium statistical mechanics, on which it is mainly based on. (i) One of the postulates, *Ergodic hypothesis* says if a system evolves freely over long enough period of time it will explore all the possible configuration available to it and spends equal amounts of time in each configuration. In other words, both the descriptions of averaging discussed above are equivalent. (ii) Second postulate is *apriori probability* that says all the accessible microstates compatible for a given macrostate are equally probable. (iii) The third one is Boltzmann's hypothesis that relates the entropy of a system to the probability of its microscopic configuration. It states that in an isolated system in thermodynamic equilibrium, the most probable distribution of microscopic states is one that maximizes the entropy of the system, subject to any constraints that may exist. If a trajectory fills the space by a hypervolume ω in the phase space, then the system entropy is defined as $S = kln\omega$, where k is the Boltzmann's constant Pathria (1996); **?**. Boltzmann's relation provides a link between macroscopic properties of the system such as its temperature and pressure and microscopic behavior of its constituent particles means a bridge between thermodynamics and statistical mechanics while the ergodic hypothesis ensures that the system is internally consistent Pathria (1996); Zemansky & Dittman (1997).

There are systems that come under the category of nonequilibrium systems due to the different phenomenologies they exhibit and so they do not follow the usual formalism of equilibrium statistical mechanics. One of the phenomena is collective behavior that ranges from small microscopic scale starting from few nanometers to large macroscopic scale like upto few meters, and is observed in many natural systems for example, bacterial colonies Costerton et al. (2005); Dombrowski et al. (2004a); Flemming (2002) animal herds Couzin et al. (2005), fish schools Katz et al. (2011), birds flocks[Ballerini et al. (2008a)] , collection of cytoskeletal filaments [Ahmadi et al. (2006); Hubbard S. (2004)] such as microtubules Sumino et al. (2012); Surrey et al. (2001a) and molecular motors, such as myosin Joanny et al. (2007); Kron & Spudich (1986); Kruse & Jülicher (2000, 2003); Kruse et al. (2001, 2004b); Kruse et al. (2005b) etc. The progress to understand the collective behavior of such systems is being significantly made through various remarkable studies done in last few decades. Understanding the broad range of nonequilibrium phenomena in terms of statistical mechanics as well as their thermodynamics is an interesting area of current research. The nonequilibrium system may arise due to the exchange of energy, matter or both with their sorroundings that leads to exhibit temporal variations in their macroscopic properties. Such systems do not follow time reversible symmetry and principle of detailed balance. These properties lead to the presence of non zero fluxes or currents in the systems. Based on some common properties, the nonequilibrium systems can be categorized in different classes. One such class of nonequilibrium systems includes the systems with infinitely slow relaxation towards thermal equilibrium, e.g. relaxation of glasses. Another class may consists the systems with presence of non-zero steady current which leads to bulk dynamics of the system and prevent them attaining the equilibrium. One such examples can be understood from heat flow experiments in which a piece of matter is connected with multiple reservoirs held at different temperatures. The third class of nonequilibrium systems includes living objects or 'active matter' system Bechinger et al. (2016); Bendix et al. (2008); Dombrowski et al. (2004a); Marchetti et al. (2013); Peruani et al. (2012); Rafaï et al. (2010); Ramaswamy (2010); Szabó et al. (2006); Toner et al. (2005a), in which the energy is injected at each particle level and dissipated energy is not correlated with the input. This thesis mainly focuses on active matter, which we are going to discuss in details in the following section.

1.3 Active matter systems: A class of nonequilibrium systems

As the name suggests, active matter systems is a class of nonequilibrium system that includes living or active objects and abundant in nature. Such system ranges from micron size e.g. bacteria, biological cells, ingredients inside the cells to macro-size organisms like animal herds, fish schools and birds flocks etc. Active matter systems are composed of large number of active or self- propelled particles where each constituent in the matter is able to take energy from the environment and convert this energy into some systematic motion, often in collection. The interaction of active particles with each other, and with the medium they live in, gives rise to highly correlated collective motion. Since the energy in active matter is consumed on each constituent level, that makes it complicated to track the amount of consumed energy and amount of converted energy into persistent motion. So underlying physics behind this behavior is not simple and physics of equilibrium system or time dependent energy functions can not be used to study the properties of such systems. It leads us to use the tools of nonequilibrium statistical mechanics in active matter and active matter can be classified as a sub-branch of nonequilibrium statistical mechanics. Apart from the natural active matter, there are artificially designed active systems, e.g. active colloids Bricard et al. (2013); Theurkauff et al. (2012), active polar disks Deseigne et al. (2010), vibrated granular rods Blair et al. (2003b); Kumar et al. (2014); Narayan et al. (2007) etc that fall under the category of active matter. They are good laboratory designed experiments to study the properties of active matter systems. We will mainly focus on the dynamics, kinetics and statistics of active matter in this thesis.

Due to energy injection at each particle level, active systems are not similar to other out of equilibrium systems like a bulk fluid sheared from the top [Saracco et al. (2011); Saracco et al. (2012)] or driven diffusive systems [Balakrishnan (2021)]. However a nonequilibrium steady state (NESS) can be defined for active matter similar to other out-of-equilibrium systems [Balakrishnan (2021)]. For the true equilibrium systems, we define the steady state when the macroscopic properties statistically remain unchanged with time, whereas for nonequilibrium systems the steady state is defined when the relevant macroscopic observables statistically remain the same with time. We can understand NESS with an example of a bird flock or fish school where all the agents (bird/fish) move coherently so we can consider this arrangement as steady state with a non zero steady particle current that tells us the violation of principle of detailed balance.

To understand the principle of detailed balance, let us consider, the probability $P(A,t)$ of finding the system in a microscopic state A at time t. The time evolution of probability $P(A,t)$ is given by the master equation,

$$\frac{dP(A,t)}{dt} = \sum_{A' \neq A} \Omega(A' \to A)P(A',t) - \Omega(A \to A')P(A,t), \tag{1.1}$$

where, $\Omega(A' \to A)$ represents the rate of change of transition from configuration A' to A. In the steady state, $P(A,t)$ is no longer function of time hence left hand side (L.H.S). of the Eq ~1.1 will vanish, and the probability $Q(A,t)$ of the system going from configuration A to A', ($Q(A,t) = \Omega(A \to A')P(A,t)$) is equal to the probability $Q(A',t)$ of the system going from A' to A, ($Q(A',t) = \Omega(A' \to A)P(A',t)$). Hence the condition of detailed balance is satisfied. That ensures that the system reaches to its steady state. However in the active matter there is a persistent flow of energy in the steady state of the system that shows the violation of detailed balance.

Large density fluctuation in the steady states of active matter is an another significant feature of active matter, which makes it different from the steady states of equilibrium systems. For an equilibrium system, for a region of volume V, containing N number of particles, the system shows fluctuation with standard deviation $\Delta N \propto \sqrt{N}$ provided the system is not close to the critical point. Whereas for an active system, the density fluctuations grow faster than usual $\sqrt{N}$ and in two dimensions, it can also grow as large as N in many cases [Ramaswamy et al. (2003a); Toner et al. (2005b)]

1.4 Classification of active matter system

Active particles are generally elongated and their own anisotropy is dominant for the direction of their self propulsion rather than an external field. Thus orientational order is a feature that is defined through much of the active matter narrative. Emergent structure with collective behavior, pattern formation, nonequilibrium order-disorder transition are some of the captivative properties exhibited by active matter Cates et al. (2008); Giomi et al. (2010); Mishra & Ramaswamy (2006); Ramaswamy & Simha (2006). Due to the overall complexity of active matter, a theoretical description to explain all properties of an active system is not fully developed. So, understanding the dynamical organization and motion of living system is first step towards developing a simple theoretical description for active systems. There are many macroscopic properties of active matter system that are universal that means even though these systems operate at different length scales with different microscopic dynamics, they show broadly similar properties. For e.g. flocking phenomena are seen in fish shoals [Parrish & Hamner (1997)] and collections of keratocytes [Szabó et al. (2006)] . Contractile stresses are evident on a subcellular scale in the cytoskeleton [Bendix et al. (2008); Joanny & Prost (2009)] as well as on a scale of many cells in swimming algae[Rafaï et al. (2010)]. These properties make us able to classify active matter in a small number of universality class, each with a well defined macroscopic behavior. So based on the consideration of symmetry and conservation laws, there are mainly four classes of active matter mentioned as follows:

1.4.1 Polar, apolar and active Brownian particles

Polar active systems are in general elongated self-propelled objects, in which their heads and tails can be distinguished [Jolles et al. (2018); Sumpter et al. (2008)]. While apolar objects do not distinguish between heads and tails [Ahmadi et al. (2005, 2006). Polar ordered phase and nematic ordered phase describe ordering in polar active matter. When all the microscopic objects align on an average in the same direction, they exhibit the polar ordered phase defined by a vector order parameter, P, known as polarisation. On the other hand, if polar self-propelled objects are oriented parallelly with random head-tail orientation, then they show nematic ordering. Apolar objects don't have polarity and exhibit nematic ordering only with parallel orientation and symmetry in their heads and tails. Nematic ordering is defined by a tensor order parameter, Q, known as alignment tensor. There is another interesting class of self-propelled objects, which are symmetric in shape and can be distinguished from their head and tail during their motion [Bialké et al. (2012); Farrell et al. (2012); Fily & Marchetti (2012); Redner et al. (2013b); Solon et al. (2015a)]. Such class of self-propelled particles is known as active Brownian Particles (ABPs). Fig 1.1 (a), (d) and (f) show the polar, apolar and active Brownian particle and (b), (c), (e) and (g) represent the different ordering they exhibit in the system.

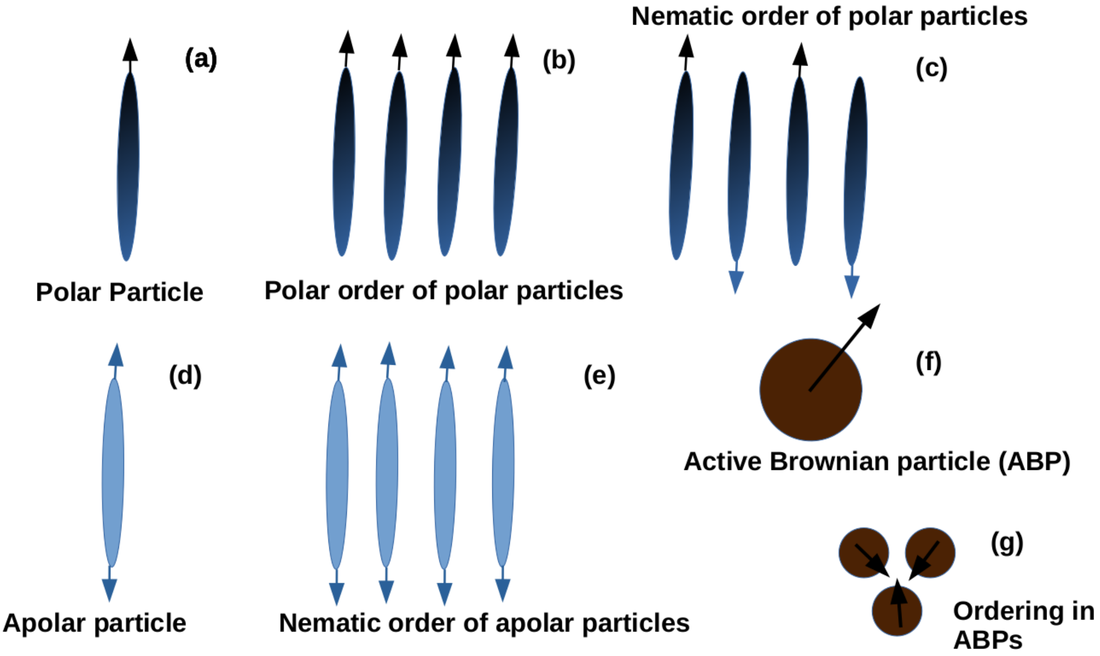

Fig. 1.1 (color online) Schematic diagram shows the polar,apolar and active Brownian particle and the different ordering exhibited by them. Arrow shows their direction of self propulsion. Head and tail symmetry is depicted by double arrows.

1.4.2 Dry and wet active system

The systems in which the collection of active particles transfer their momentum to the fluid medium, due to the friction provided by the fluid medium are known as $'dry'$ systems in which the momentum conservation is violated. Examples of such natural dry systems are bacteria gliding on a rigid surface [Wolgemuth et al. (2002)], animal herds on land [Toner & Tu (1998)] or artificially designed active systems such as vibrated granular particles on a two-dimensional substrate [Blair et al. (2003a); Kudrolli et al. (2008a); Ramaswamy (2017); Ramaswamy et al. (2003a); Yamada et al. (2003)]. Furthermore, there are some examples like systems of concentrated swimming bacteria [Drescher et al. (2011)] , motor filament suspension [Liverpool (2003)] where the steric and random fluctuation suppress the hydrodynamic interaction. The only conserved quantity in a dry system is the number of particles (neglecting birth and death) and the associated hydrodynamic field is the local density and orientation of active particles. On the other hand, when the particles are suspended in a fluid medium and the solvent-mediated hydrodynamic interaction are taken into account, the systems are modeled by incorporating the dynamics of suspending fluid medium and developing a description of suspension of active particles and fluid medium, such systems are known as $'wet'$ systems with conserved total momentum.

We can summarize the classification of active matter through various examples that categorically discuss the $'dry'$ and $'wet'$ with polar and nematic interaction. Examples of dry polar systems are animal herds [Parrish & Hamner (1997)], cell layers [Serra-Picamal et al. (2012)], vibrated asymmetric granular particles [Kudrolli et al. (2008b)], films of cytoskeletal extracts [Surrey et al. (2001a)], dry nematic systems are melanocytes [Kemkemer et al. (2000)], vibrated granular rods [Narayan et al. (2007)], wet polar systems are cell cytoskeleton and cytoskeletal extracts in bulk suspensions [Bendix et al. (2008)], swimming bacteria in bulk [Dombrowski et al. (2004b)] and wet nematic systems are suspensions of catalytic colloidal rods [Paxton et al. (2004a)] etc. Our study mainly focuses to discuss the ABPs and wet polar active matter.

1.5 Methodology

To understand and characterise the different complex and fascinating behavior exhibited by active matter, various studies have been done. Due to non conservation of energy in such systems, it is not possible to write an effective Hamiltonian to explain their behavior. So in last couple of decades, there are enormous studies that have focused on following three approaches to study active matter systems: (i). microscopic rule based study like Vicsek model/agent based simulation [Grégoire & Chaté (2004a); Vicsek et al. (1995) (ii). hydrodynamic equations of motion written for the coarse grained hydrodynamic variables like density and order parameter fields and (iii) using experimental techniques [Paxton et al. (2004b)] that have given more insight about these systems.

Now we are going to discuss these methods in details and then we will emphasize the approaches and the properties that we have opted for our studies:

1.5.1 Agent-based simulation

The approach of agent-based simulation defines the modelling of system in two ways: (i) microscopic rule-based simulation, e.g. Vicsek model [Vicsek et al. (1995)] (ii) Langevin's equation of motion. A simulaion technique that aims to model and simulates the behavior and interaction of individual entities based on predefined rules and conditions is what we know as microscopic rule-based simulation. In this type of simulation, the focus is on the behavior and actions of individual components within a system rather than on aggregated or macro-level effects. In this simulation, each agent or entity within the system is defined with specific characteristic, behaviors and rules that govern their interaction with other agents and the environment and the positions and velocities of the entities are updated through the dynamical equations based on these rules. The phenomenology of the concerned active system works as base to define the update rules. Active shape asymmetric agents move along their long body axis. For finite size particles alignment with their neighbors in contact is guided by the volume exclusion [Chaté et al. (2008a); Fily & Marchetti (2012); Pattanayak et al. (2019a); Shi & Ma (2013)]. For polar agents the interactions work like "ferromagnetic" interaction in spin systems and for apolar agents both parallel and anti-parallel interactions are possible. Agents are considered as point particles in number of studies, but alignment interactions (polar/apolar) are kept by hand to mimic the alignment due to the finite size of the agents [Grégoire & Chaté (2004a); Vicsek et al. (1995)]. Appropriate noise terms are used in the update rules to take the errors, made by active agents while interacting with their neighbors Grégoire & Chaté (2004a); Vicsek et al. (1995). Another agent-based technique is what we know as Langevin's equation of motion. It models the dynamics of individual agents or particles incorporating both deterministic and random components to describe the agent's motion or behavior. It is used to model the active Brownian particle by adding one more term to describe an active system to Langevin's equation called the "active" term or the "activity".

Vicsek Model: A rule based model

A minimal rule-based model was introduced by [Vicsek et al. (1995)] in order to investigate the emergence of self-ordered motion in systems of self -propelled polar particles (fish school and bird flocks). This work addresses the clustering, transport, and phase transition in nonequilibrium systems where the velocity of the particles is determined by a simple rule and random fluctuations. The model is a transport related, nonequilibrium analog of the ferromagnetic type of models, with the important difference lies in its novel type of dynamics. The Vicsek model [Vicsek et al. (1995)] is defined in two-dimensions where each SPP in the system is described as a point-particle with a direction θ_i at time t, moving continuously (off lattice) on the plane along its direction with speed v_0 and interacts with its neighboring particles with a fixed rule within an interaction radius, r. At every time step, an alignment rule works for each particle i as follows: (i) first one computes the average direction of velocities of all the particles within a circle of interaction radius r, sorrounding the given particle i. (ii) then the direction of the particle θ_i is set equal to the angle correspondent to this average direction, with an additional noise term. The polar order forms via head-to-head alignment of particles. The direction, velocity and position updates resulting from the ’aligning rule’ at discrete time step, Δt are given as:

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t+\Delta t)\Delta t \tag{1.2}$$

$$\mathbf{v}_i(t+\Delta t) = \big(\cos(\theta_i(t+\Delta t)), \sin(\theta_i(t+\Delta t))\big) \tag{1.3}$$

and

$$\theta_i(t+\Delta t) =< \theta(t) >_r + \eta \Delta\theta \tag{1.4}$$

where equations 1.2 and 1.4 are the positions and orientation updates respectively. Here $\mathbf{r}_i$, $\mathbf{v}_i$ and θ_i are the position, the self-propulsion speed and the orientation of the i^{th} particle. $< \theta(t) >_r$ is the mean orientation of the particles within an interaction radius r. Δt (fixed) is the step-size for the update in time. $\Delta\theta \in (\pi, \pi)$ is the random noise in the alignment and $\eta \in [0,1]$ is the noise strength. The second term in eq 1.4 is “angular noise” and it applies to each particle such that it rotates it by some small angle from its original direction.

The two control parameters in the Vicsek model are mean density ρ, i.e. the number of particles per unit area, and the noise strength η. Tuning these two parameters give nonequilibrium order-disorder transition. Different exponents are observed near the phase transition as in the equilibrium counterparts. Different limits of η and ρ, turn the collective motion of particles in three ways; (i) for small ρ and η, the particles tend to form groups moving coherently in random directions, (ii) at higher densities and noise the particles move randomly with some correlation, and the most interesting case is (iii) for higher density and small noise, when particles tend to align in spontaneously selected direction , driving the whole system into an ordered flocking state. They also observed the order-disorder phase transition and the transition is continuous. Also different critical exponents are estimated analogous to equilibrium systems undergoing the phase transition.

There was still a discussion about the nature of order-disorder transition of polar SPPs. In 2004, Chate and collaborators [Chaté et al. (2008a); Grégoire & Chaté (2004a)] introduced another type of noise, called 'vector' noise. In the standard Vicsek model, the thermal noise is introduced as scalar, which means first the agent finds the mean of its neighbors and then decides its new direction with small fluctuation from the resultant direction.But in the vector noise case, the agent's new direction is decided by the resultant of mean of neighbors direction and thermal fluctuation. Mathematically the two types of noises have some differences, but on macroscopic scale their results are the same. So the influence of vector noise depends upon the local alignment and it decreases with increasing local order. Also it is found that for angular noise the nature of the order disorder transition becomes discontinuous provided one considers large enough system size because as finite size effect is much more dominant for angular noise [Foffano et al. (2012); Vicsek et al. (1995)] as compared to the vectorial choice [Grégoire & Chaté (2004b)]. In various studies the nature of the transition depends on the update mechanism of the system Aldana et al. (2007). Now, it is believed that the density phase separation is the key to make the transition first order Pattanayak & Mishra (2018); Solon et al. (2015a). But still there is need of experiments to settle the debate about the nature of the phase transition.

Langevin's dynamics

The chaotic perpetual motion of a passive particles suspended in a fluid medium is the result of its collisions with the molecules of the surrounding fluid. Such motion is called Brownian motion and suspended passive particles are called Brownian particles. The theory of Brownian motion is perhaps the simplest approximate way to treat the dynamics of equlibrium as well as nonequilibrium systems. There exists a relation between frictional forces provided by the sorrounding fluid medium and random forces due to collision of suspended brownian particle with sorrounding fluid medium. The fluctuation-dissipation theorem, FDT gives a balance between these two forces and relates these forces to each other [Pathria (1996); Zemansky & Dittman (1997)]. Newtonian dynamics describes the dynamics of passive particles which includes random and frictional forces [Romanczuk et al. (2012a)]. Hence, the equation of motion for Brownian particle of mass m suspended in fluid medium can be written by Langevin dynamics,

$$m\frac{d\mathbf{v}}{dt} = -\gamma\mathbf{v} - \nabla U(\mathbf{r}) + \eta(t) \tag{1.5}$$

Here γ is the Stokes frictional coefficient and $U(r)$ is a position dependent potential. η(t) is a random force with mean zero and satisfies the relations $\langle\eta(t)\rangle = 0$, and $\langle\eta_i(t)\cdot\eta_j(t)\rangle = 2D_b\delta_{i,j}\delta(t-t')$, where the components $\eta_i(t)$ and $\eta_j(t)$ are referred to as Gaussian white noise with intensity D_b. The indices i and j correspond to the Cartesian coordinates. The intensity D_b and friction coefficient γ are related by the FDT, $D_b = \gamma k_\beta T$ [Pathria (1996); Zemansky & Dittman (1997)] in the equilibrium where k_β and T represent the Boltzmann constant and temperature of the system respectively.

Now, when we include the active nature of the particles, it makes the Brownian particles to be called as active Brownian particles and leads to the motility induced phase separation

(MIPS) even without having any alignment interaction due to its shape symmetry [Buttinoni et al. (2013a); Cates & Tailleur (2015a); van Damme et al. (2019)]. The Langevin equation 1.5 is a second-order stochastic differential equation which includes an inertial term $m\frac{d\mathbf{v}}{dt}$ and a damping term $\gamma\mathbf{v}$. In different systems like granular systems or living organisms, the momentum dissipation caused by the friction provided by the medium is such high that the first term of Eq $\sim$ 1.5 can be neglected in the overdamped limit as motion of ABPs ceases on a very short time in this limit. Hence the dynamics of the ABP in the overdamped regime is given by the following equations:

$$\partial_t \mathbf{r}_i = v_0 \mathbf{n}_i + \mu \sum_{j \neq i} \mathbf{F}_{ij} + \eta_i^T(t) \tag{1.6}$$

$$\partial_t \theta_i = \eta(t), \tag{1.7}$$

where ABPs are taken as disk of radius a, and they interact with a soft repulsive potential that takes care of steric effects. The direction of motion of the ABP is defined by unit vector $\mathbf{n}_i = \big(\cos(\theta_i), \sin(\theta_i)\big)$, where θ_i is the orientation of the i^{th} particle. The first term in the right hand side (R.H.S) of Eq $\sim$1.6 is due to self-propelled nature of the ABP, and v_0 is the self-propulsion speed of the particle. $\eta_i^T(t)$ shows translational Gaussian white noise with mean zero and correlations $\langle \eta_{i\alpha}^T(t) \cdot \eta_{i\beta}^T(t') \rangle = 2D\delta_{ij}\delta_{\alpha\beta}\delta(t-t')$, where α,β denotes Cartesian coordinates and diffusion constant $D = \mu k_\beta T$. $\eta(t)$ is a Gaussian white noise with zero mean and correlations $< \eta(t) \cdot \eta(t') >= 2\Lambda_r \delta_{ij} \delta(t-t')$, Λ_r is the rotational diffusion coefficient and μ is the mobility. $\mathbf{F}_{ij}$ is short-range repulsive force between i^{th} and j^{th} particle. The form of $\mathbf{F}_{ij}$ considered in the study of [Fily & Marchetti (2012)] is $\mathbf{F}_{ij} = -k(2a - r_{ij})\mathbf{n}_{ij}$ if $r_{ij} < 2a$ and $\mathbf{F}_{ij} = 0$ otherwise. In another study of ABP, Stark et al. consider the Weeks-Chandler-Andersen (WCA) potential as a soft repulsive potential between the ABP [Fily & Marchetti (2012); Zeitz et al. (2017)]. General properties of the ABPs should be independent of the specific form of the considered repulsive potential. In our study in chapter 2, we have considered soft repulsive potential to study the mixture of active and passive Brownian particles.

1.5.2 Phenomenological approach : hydrodynamic equations of motion

In previous sections, we have discussed the agent-based simulation that is based on the microscopic details of the system to study the active matter. In this section we will discuss about hydrodynamic equations of motion where we write the equation for slow variables like density and orientation fields in a coarse-grained description. Hydrodynamic theory is based on the fundamental axioms of conservation laws like conservation of mass, conservation of momentum and conservation of energy, etc and the terms are written on the basis of underlying symmetry of the considered system. One way to obtain the hydrodynamic theory is to directly write hydrodynamic equations for microscopic fields, including all terms allowed by the symmetry as Toner and Tu [Toner & Tu (1995, 1998)] did for the dry flocks. Further, this approach can be extended for the suspension of SPPs in a fluid [Simha & Ramaswamy (2002a)] and active filaments solution [Hatwalne et al. (2004). The effective continuum theory for flocking was first introduced by Toner and Tu in 1995 [Toner & Tu (1995, 1998)]. This model was formulated for dry active system on the basis of symmetry considerations. For a system of self-propelled particles moving on a dry frictional substrate, the only conserved quantity is the density of active particles $\rho(r,t)$ (where the death and birth of SPPs are not included). The polar order parameter is the polarization vector field $\mathbf{P}(\mathbf{r},t)$ that defines the ordering for polar particles. The coarse-grained density $\rho(\mathbf{r},t)$, and polarisation vector field $\mathbf{P}(\mathbf{r},t)$ are defined by,

$$\rho(\mathbf{r},t) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i(t)) \tag{1.8}$$

$$\mathbf{P}(\mathbf{r},t) = \frac{1}{\rho(\mathbf{r},t)} \sum_{i=1}^{N} \mathbf{n_i} \delta(\mathbf{r} - \mathbf{r}_i(t)) \tag{1.9}$$

where the summation is over all the particles, $\mathbf{r}_i(t)$ and $\mathbf{n}_i(t)$ are the position and the unit orientation vector of i^{th} particle at time t.

and the hydrodynamic equations of motion are given as

$$\partial_t \rho(\mathbf{r},t) + v_0 \nabla \cdot (\rho \mathbf{P}) = -\nabla \cdot \big(-\frac{1}{\gamma_\rho} \nabla \frac{\delta F(P,\rho)}{\delta \rho} + \mathbf{f}_\rho \big) \tag{1.10}$$

$$\partial_t \mathbf{P} + \lambda_1 (\mathbf{P} \cdot \nabla) \mathbf{P} = -\frac{1}{\gamma} \frac{\delta F(P,\rho)}{\delta \mathbf{P}} + \mathbf{f} \tag{1.11}$$

where $F(P,\rho)$ is a free energy functional that includes the interaction among the particles, γ_ρ, γ are kinetic coefficients, and v_0 is the self-propulsion speed of the active particles. The first term on the right hand side (R.H.S) of Eq $\sim$ 1.10 yields a familiar diffusive current, and $\mathbf{f}_\rho$ is the associated noise. The second term in the left hand side (L.H.S) of Eq $\sim$ 1.10 represents the active current, which is proportional to the self-propulsion speed v_0. Advection present in the system is taken care by considering the advective term analogous to the famous Navier-Stokes equation for fluids. λ_1 depicts the strength of the advective term in Eq $\sim$1.11. In active flocks, the strength of the advective term λ_1 is a phenomenological parameter that can be determined from a microscopic model as here the the constraint of Galilean invariance does not hold for motion of the particles. Here $\mathbf{P}$ denotes both a velocity field and a local orientation order parameter of the system. Therefore, $\mathbf{P}$ introduces a term for advection and flow alignment in Eq $\sim$ 1.11, and $\mathbf{P}$ acts as only a velocity field in Eq $\sim$ 1.10. The last term on the right-hand side (R.H.S) in Eq $\sim$ 1.10 includes the fluctuations in the system, which is a Gaussian white noise with zero mean and correlations such that,

$$\langle f_i(\mathbf{r},t) f_j(\mathbf{r}',t')\rangle = 2\Delta\delta_{ij}(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{1.12}$$

where Δ is a constant and dummy indices i, j represents cartesian components. The considered noise in Eqs $\sim$ 1.10, 1.11 is purely additive that means it is independent of order parameter $\mathbf{P}$ and local density ρ. As it is discussed for active systems , $\mathbf{P}$ plays dual role, (i) $\mathbf{P}$ is the orientational order parameter of the system, and (ii) $v_0\mathbf{P}$ represents the velocity field. This dual behavior of $\mathbf{P}$ is significant in determining the large-scale behavior of these systems. The free-energy functional used in Eqs $\sim$1.10 and 1.11 is given as

$$F(P,\rho) = \int_r [\frac{\overline{\alpha}(\rho)}{2}|\mathbf{P}|^2 + \frac{\overline{\beta}}{4}|\mathbf{P}|^4 + \frac{\overline{K}}{2}(\partial_l P_m)(\partial_l P_m) + \frac{\omega}{2}|\mathbf{P}|^2\nabla\cdot\mathbf{P} - \omega_1\nabla\cdot\mathbf{P}\frac{\partial\rho}{\rho_0} + \frac{A}{2}(\frac{\delta\rho}{\rho_0})^2], \tag{1.13}$$

where ρ_0 is the mean density of the system, and $\delta\rho = \rho - \rho_0$ represents the fluctuation in density around its mean value ρ_0. The first two terms of right hand side in Eq $\sim$1.13 describe the mean-field order-disorder transition of the system. $\overline{\alpha}(\rho)$ is a microscopic model-dependent parameter, which depends on local density ρ and noise strength [Bertin et al. (2006)]. $\overline{\alpha}(\rho)$ fluctuates around zero near to the critical point, and shows negative value in the ordered state. $\overline{\alpha}(\rho)$ can be defined phenomenologically to describe the physics near the transition as, $\overline{\alpha}(\rho) = a_0(1-\frac{\rho}{\rho_c})$ where a_0 is a positive constant and $\overline{\alpha}(\rho)$ changes sign at $\rho = \rho_c$. $\overline{\beta} > 0$ is a stabilisation factor for the system that is positive. In the ordered state, these two parameters make the non-zero value of order parameter, $|\mathbf{P_0}| = \sqrt{\frac{\alpha_0}{\beta}}$, where $\alpha_0 = \alpha(\rho_0)$. In Eq $\sim$1.13, the third term represents the energy cost due to spatially inhomogeneous deformations of the coarse-grained order parameter and the Franks constant, $\overline{K}$ is positive. Splay and bend in the order parameter are also taken care by this and all three elastic constants are taken the same. The deformations play a significant role in the active systems [Voituriez et al. (2006)]. Further, ω terms can be considered as correction to $\overline{\alpha}(\rho)$ due to splay. The suppression in the density fluctuation is represented by the last term and A shows the compression modulus. Now, using the free energy functional $F(P,\rho)$ of Eq ~1.13, the hydrodynamic equation of motion of $\mathbf{P}$ takes the form,

$$\partial_t \mathbf{P} + \lambda_1 (\mathbf{P}\cdot\nabla)\mathbf{P} = -\left[\alpha(\rho) + \beta|\mathbf{P}|^2\right]\mathbf{P} + K\nabla^2\mathbf{P} - v_1 \nabla \frac{\rho}{\rho_0} + \frac{\lambda}{2}\nabla|\mathbf{P}|^2 - \lambda\mathbf{P}(\nabla\cdot\mathbf{P}) + \mathbf{f}, \tag{1.14}$$

where $v_1 = \frac{\omega_1}{\gamma}$ and $\lambda = \frac{\omega}{\gamma}$ and both have the dimensions of velocity and the quantities $\alpha = \frac{\overline{\alpha}}{\gamma}$ and $\beta = \frac{\overline{\beta}}{\gamma}$. In polarisation (**P**) Eq ~1.14 can be compared to the *Navier-Stokes equation* for a fluid where the polarisation **P** is generally proportional to the flock velocity. The second term of the right-hand side of Eq ~ 1.14 represents the viscous force. The third and fourth term represent an approximate form of pressure gradient gradient $-\frac{1}{\rho}\nabla P$, where considering to the leading order $P(\rho) \approx v_1 \rho$ which shows the similarity with *Navier-Stokes equation*. Two more important terms based on symmetry argument include hydrodynamic equation for **P** viz; $(\frac{\lambda_3}{2})\nabla|\mathbf{P}|^2 + \lambda_2\mathbf{P}(\nabla)$ (Mishra et al., 2010; Toner & Tu, 1995).

Homogeneous steady states

A collection of polar particles show order-disorder transition that depends on the system parameters. For $\alpha > 0$ corresponding to $\rho_0 < \rho_c$, the system is in the disordered state with order parameter $|\mathbf{P}| = \mathbf{0}$. For $\alpha < 0$ corresponding to $\rho_0 > \rho_c$, the system is in the ordered state with a non-zero value of order parameter, $|\mathbf{P_0}| = \sqrt{\frac{\alpha_0}{\beta}}$, where $\alpha_0 = \alpha(\rho_0)$, the order moving state, with velocity $\mathbf{v} = v_0\mathbf{P}_0$. The continuous rotational symmetry of the system is spontaneously broken in the ordered state.

1.6 Coarsening

Previous sections were focused on different features of a collection of self-propelled particles observed in steady state like collective motion, pattern formation or giant number fluctuation and their equations of motion are discussed through different approaches. In the present section, we will talk about a fascinating class of problem, in which the study is about the dynamical process through which a system evolves from one phase to another phase depending upon the range of parameters. This class of problem involves the kinetics of phase transition or phase-ordering kinetics or coarsening. To understand this class of problem we can think of the systems that exhibit multiple phases depending upon the value of the external set of parameters like temperature, pressure etc. For a given set of parameters the system chooses to stay in a particular state that corresponds to the minimisation of its free energy. For e.g let's consider a system is in its solid state, and we rapidly change the temperature to the value where its preferred equilibrium phase is liquid. The system will take some time to convert from solid to liquid. The initial and the final states are understood by the properties of the corresponding equilibrium state, but understanding of the dynamical process through which it goes from solid to liquid phase is is not much known. Although there have been studies over the years which has helped us in our basic understanding of such dynamical processes Bray (1994); Puri (2004). Now we will first focus on discussing the kinetics or coarsening of systems where system approaches to an equilibrium state, and then we will describe coarsening in the active matter systems.

1.6.1 Coarsening in systems with nonconserved kinetics (Model A)

To understand the coarsening in systems with nonconserved kinetics, we can think of magnetic systems. Let's start considering the case of ferromagnet with zero magnetic field. At high temperature, ($T > T_c$) the system is in disordered or paramagnetic state.

Now, upon rapidly quenching the temperature below the critical value, T_c, the systems reaches to its preferred magnetized state, which is characterised by emergence and growth of domains enriched in either "up" or "down" spins. The coarsening of the domains is characterized by a characteristic domain length $L(t)$, and a finite system will order either with all up or down state at large time. We will see this coarsening in Ising model, which is the most simple model and first introduced as a model to study the phase transition in magnetic systems Plischke & Bergersen (1994). In the Ising model spins can have either up ($S_i = +1$) or down ($S_i = 1$) orientation. Now kinetics can be associated with the Ising model by assuming a heat bath connected with the system to generate stochastic spin flips ($S_i \to -S_i$). This random spin flip model is known as spin-flip or Glauber model Glauber (1963) where the corresponding order parameter of the system is non-conserved.

Now we need an appropriate order-parameter to describe the system at coarse-grained level which is local magnetisation $\psi(\mathbf{r},t)$ in this system. The evolution of the order parameter is governed by time-dependent Ginzburg landau equation (TDGL). So the dynamical equation for the local magentisation, $\psi(\mathbf{r},t)$ takes the form

$$\frac{\partial \psi(\mathbf{r},t)}{\partial t} = -\Gamma_0 \frac{\delta \mathscr{F}_l[\psi]}{\delta \psi(\mathbf{r},t)} + \theta(\mathbf{r},t) \tag{1.15}$$

where Γ_0 is the inverse damping coefficient and $\frac{\delta \mathscr{F}_l[\psi]}{\delta \psi(\mathbf{r},t)}$ is the functional derivative of free-energy functional where the free-energy functional $\mathscr{F}_l[\psi]$ is defined as

$$\mathscr{F}_l[\psi] = \int d^d r \{g(\psi(\mathbf{r},t)) + \frac{K}{2} |\nabla \psi(\mathbf{r},t)^2|\} \tag{1.16}$$

Where $g(\psi(\mathbf{r},t)$ is the Landau free energy and second term accounts for the surface tension due to the inhomogeneity in the order parameter and K is strength of the surface tension. We have used the general form of ψ^4 free energy:

$$\mathscr{F}_l[\psi] = \int d^d r\{-\frac{1}{2}a(T_c - T)\psi(\mathbf{r},t)^2 + \frac{K}{2}|\nabla\psi(\mathbf{r},t)^2| + \frac{b}{4}\psi(\mathbf{r},t)^4\} \tag{1.17}$$

where, $a < 0$ shows the broken symmetry state, $b > 0$ is a stabilisation factor and T_c is the critical temperature in the system. Using the expression for ψ^4 free energy and introducing rescaled variables in eqn 1.15 one can obtain dimensionless time dependent Ginzburg landau (TDGL) equaion

$$\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \psi - \psi^3 + \nabla^2\psi + \theta(\mathbf{r},t) \tag{1.18}$$

where $< \theta(\mathbf{r},t) >= 0$ and $< \theta(\mathbf{r},t)\theta(\mathbf{r}',t') >= 2\xi\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$ and ξ is given as $\xi = \frac{k_B T b[a(T_c-T)]^{(d-4)/2}}{K^{d/2}}$, to make the whole equation dimensionless.

1.6.2 Coarsening in systems with conserved kinetics (Model B)

When a system evolves from homogeneous phase to ordered phase and in the evolution the associated order parameter is conserved, such systems are studied under the conserved kinetics. To understand the kinetics of such system we take an example of phase separation in binary mixture. If we have a AB binary mixture and we quench it from homogeneous phase to segregated phase, then the segregation happens by formation and growth of domain enriched with either A or B type species and at late times both A and B will be completely phase separated. The dynamics in this case is different from the nonconserved case. The atoms diffusion takes place and they exchange their sites simultaneously with another atom. So unlike the spin flip this model involves the spin exchange that is the spin S_i jumps from $+1$ to -1 while a neighbor S_j simultaneously jumps from -1 to $+1$ and the resultant model is called Kawasaki model Kawasaki (1966).

For the conserved case, the appropriate space-time dependent order parameter to describe the system is difference in densities of A and B species (relative density of the system). So the order parameter is given as $\psi(\mathbf{r},t) = n^A(\mathbf{r},t) - n^B(\mathbf{r},t)$ where $n^A(\mathbf{r},t)$ and $n^B(\mathbf{r},t)$ are the local densities of species A and B respectively. The evolution dynamics of $\psi(\mathbf{r},t)$ is given by the continuity equation

$$\frac{\partial}{\partial t}\psi(\mathbf{r},t) = -\nabla\cdot\mathbf{J}(\mathbf{r},t) \tag{1.19}$$

where $\mathbf{J}(\mathbf{r},t)$ denotes the current, which is given as

$$\mathbf{J}(\mathbf{r},t) = -D\nabla\mu(\mathbf{r},t) \tag{1.20}$$

D is diffusion coefficient and $\mu(\mathbf{r},t)$ is the chemical potential. The chemical potential is given by

$$\mu(\mathbf{r},t) = \frac{\partial\mathscr{F}[\psi]}{\partial\psi(\mathbf{r})} \tag{1.21}$$

where $\mathscr{F}[\psi]$ is the free energy. Combining all those above equations we get the Cahn-Hilliard-Cook (CHC) equation which models the phase separation in binary mixture and given as:

$$\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \nabla\cdot[D\nabla\frac{\delta\mathscr{F}[\psi]}{\delta\psi} + \theta(\mathbf{r},t)] \tag{1.22}$$

where D is the diffusion constant and $\mathscr{F}$ is the free energy defined in equation 1.17. Noise is defined as $<\theta(\mathbf{r},t)>= 0$ and $<\theta(\mathbf{r},t)\theta(\mathbf{r}',t')>= 2DK_BT\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$. Using the expression for ψ^4 free energy and introducing rescaled variables in eqn 1.22 one can obtain dimensionless CHC equaion

$$\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \nabla\dot{[}\nabla(-\psi+\psi^3-\nabla^2\psi)+\theta(\mathbf{r},t)] \tag{1.23}$$

where $< \theta(\mathbf{r},t) >= 0$ and $< \theta(\mathbf{r},t)\theta(\mathbf{r}',t') >= 2\xi\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$ and ξ is given as $\xi = \frac{k_B T b[a(T_c - T)]^{(d-4)/2}}{K^{d/2}}$.

1.6.3 Correlation function and structure factor

As the system evolves, it coarsens with time via the formation and growth of domains. The structural and dynamical properties of the domains are calculated by correlation function and structure factor and one introduces the characteristic length scale, $L(t)$ to characterise this growth. Correlation function and structure factor exhibit scaling properties in the system. If the morphology of domains remains unchanged with time, the system is characterised by a single length scale, $L(t)$ and the correlation function $C(r,t)$ of the order parameter shows dynamic scaling. The order parameter correlation function is given by

$$C(\mathbf{r},t) = \frac{1}{V}\int d\mathbf{R}\,[< \psi(\mathbf{R},t)\psi(\mathbf{R}+\mathbf{r},t) > - < \psi(\mathbf{R},t) >< \psi(\mathbf{R}+\mathbf{r},t) >\} = g(\frac{r}{L(t)}) \tag{1.24}$$

where $g(\frac{r}{L(t)})$ is the time independent scaling function and $L(t)$ is the characteristic length of the domain at time, t. Correlation function, being time dependent shows the dynamic scaling for the scaling function $g(x)$. We calculate the averaged correlation function, $C(r,t)$ for different realisations and averaged over different directions.

Now we obtain the growth law for nonconserved and conserved kinetics by writing down the equation of motion for the interfaces. First let's discuss about the nonconserved case. For nonconserved scalar order parameter, effective velocity of the domain wall should be equal to its curvature. For a domain of characteristic length $L(t)$, the velocity,v of domain wall is $v \sim \frac{dL}{dt}$ and the curvature of the domain, $K \sim \frac{1}{L}$. Hence, the diffusive growth law for non-conserved scalar order parameter is $L \sim t^{\frac{1}{z}}$, and $z = 2$ in this case which is known as dynamical growth exponent Allen & Cahn (1979); Hohenberg & Halperin (1977). However, for some systems we need n-component vector order parameter like polar fluid, nematic liquid crystals etc Bray (1994). In such systems, we need a logarithmic correction to discuss the power law in domain growth. The logarithmic correction for the domain growth in case of two component vector order parameter is given as, $L \sim (\frac{t}{lnt})^{\frac{1}{2}}$ Blundell & Bray (1994); Bray (1994); Mondello & Goldenfeld (1990).

For the systems with conserved order parameter the chemical potential, μ on the surface of domain of size $L(t)$, is $\mu \sim \frac{\sigma}{L(t)}$, where σ is the surface tension. So the concentration current varies as $D|\nabla\mu| \sim \frac{D\sigma}{L(t)^2}$, D is the diffusion constant. Therefore, we obtaing the growth law from the interfacial equation of motion for domain size growth, which goes as goes as $\frac{dL(t)}{dt} \sim \frac{D\sigma}{L(t)^2}$ or $L(t) \sim (D\sigma t)^{\frac{1}{z}}$, $z = 3$ in this case Lifshitz & Slyozov (1961).

Now another experimentally relevant quantity that exhibit scaling property in the system is structure factor, which is defined as the Fourier transform of real-space correlation function and given as $S(\mathbf{k},t) = \int d\mathbf{r} e^{i\mathbf{k}\dot{\mathbf{r}}} C(\mathbf{r},t)$, where $\mathbf{k}$ is the wave-vector of the scattered wave. The corresponding dynamic scaling form shown by $S(\mathbf{k},t)$ is $S(\mathbf{k},t) = L(t)^d f(kL(t)$. The scaling function is obtained as $f(q) = \int d\mathbf{r} e^{i\mathbf{q}\dot{\mathbf{r}}} g(r)$. The scaling function $g(r)$ and $f(q)$ gives the morphology of the dynamical system. The tail of structure factor shows a power law decay, given by generalised Porod's law, which says $f(kL(t)) \sim (kL(t))^{-(d+n)}$ for n-component order parameter in d-dimensions.

1.6.4 Coarsening in active systems

Coarsening in active systems takes place in the framework of their nonequilibrium steady states that makes them different from their equilibrium counterparts. It is found that coarsening in active polar and active nematic syetms show a deviation from Porod's law and also the activity shows a remarkable effect on the growth kinetics for conserved and nonconserved systems. For polar systems, governed by nonconserved kinetics Toner and Tu predicted the growth law for coarse-grained density $L_\rho(r,t) \sim t^{5/6}$ Toner & Tu (1998). For the phase separation of active Brownian particles (ABPs), the ordering kinetics, governed by conserved growth has shown a slower growth due to activity as observed in the studies Pattanayak et al. (2021a,b); R.Wittkowski & Cates (2014). In our work, we have addressed the effect of thermal noise on the coarsening of ABPs and also the relevance of hydrodynamic field on the orientational field of particles.

1.7 Organisation of the thesis

In the previous sections we have introduced active matter systems and discussed their classes based on the symmetry and conservation laws. Then we have given details of the different methodologies to study such systems. We have also discussed about the ordering kinetics and what properties we can observe to study such systems. We discuss our findings in the next chapters. Here we give a brief about the works contained in the coming chapters.

In chapter 2, we study the binary mixture of active Brownian particles (ABPs) and passive particles and aim to understand the effect of size and activity of the active particles on the growth kinetics and steady state properties of the passive particles. The system is studied on a two-dimensional substrate using overdamp Langevin dynamic simulation. We observe that large size and activity of the ABPs lead the passive particles to form periodic hexagonal close pack (HCP) spanning clusters in the system. We also study the kinetics of growing passive particle clusters and find that the mass of the largest cluster shows a much slower growth kinetics in contrast to conserved growth kinetics in ABPs system.

The Chapter 3 is about the steady state properties of ABPs in the presence of a random quenched obstacle. In this study we fix an obstacle in space and time and use the overdamp Langevin dynamics to analyse the steady state properties of the ABPs for different sizes of the obstacle and activity of the ABPs for different packing fractions of the system. We find that the obstacle enhances the phase separation in ABPs and system shows the coexistence of low density and high density regions. Further we make the phase diagram in the plane of packing fraction and activity for various sizes of the obstacle and compare it with the case when there is no such obstacle present in the system. We find that the phase boundary shifts and system developes an binodal envelop which provides the range of parameters for which the phase separated densities collapse onto a single coexistence curve. Chapter 4 addresses the role of noise on the ordering kinetics of the collection of active Brownian particles which is modeled using coarse-grained conserved active model B (AMB). The ordering kinetics of the system is studied for the critical mixture when quenched from high to low temperature.We find that the noise is relevant for the growth kinetics of AMB. We use extensive numerical study as well as dynamic scaling hypothesis and find that asymptotic growth law for AMBN is shows a crossover from 0.25 to 0.33,diffusive Lifshitz-Slyozov (LS) type. We find that two different scaling functions for intermediate time with growth exponent 0.25 and late time with growth exponent 0.33 are present in the system. Details are discussed in the chapter 4. In Chapter 5 we study the AMB with noise for off-critical composition. First we study the system when the system is slightly away from the critical mixture and further we analyse the results for deep off critical mixture. We see that for slightly off critical mixture, the system develops a competition between the activity and asymmetry due to the off-criticality present in the system. For deep off-critical mixture we find no such competition and exponent always remains 0.33. In Chapter 6 we model a collection of orientable objects suspended in fluid medium and observe the relevance of hydrodynamic field on the ordering kinetics of the orientation of the particles. The polar particles are supplied with active stresses and momentum damping coming from the viscosity of bulk fluid medium.The effect of active fluid is contractile or extensile depending upon the sign of the active stress. We explore the growth kinetics for different activities and compare it with the equilibrium nononserved kinetics (Model A). We find that for both extensile and contractile cases the growth is altered by a prefactor and the extensile fluid enhances the domain growth whereas the contractile fluid supresses it. Also

The asymptotic growth becomes pure algebraic for large magnitudes of activity.Finally in Chapter 7 we conclude our work alongwith the future interests and remarks.

1.8 Technical details

The numerical results discussed in the upcoming chapters are obtained by writing the numerical codes and simulated using the FORTRAN 77/90 compiler. Plots are generated by using the XMGrace and Gnuplot plotting tools. All the simulations are performed on the Institute clusters as well as PARAM Shivay computing facility at IIT(BHU) Varanasi India, 221005.

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