

Phase Separation in Colloids in the Presence of Activity

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*A dissertation submitted for the partial fulfillment of
BS-MS dual degree in Science*



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Certificate of Examination

This is to certify that the dissertation titled **Phase Separation in Colloids in the Presence of Activity** submitted by **Mr. Vishnu N Nampoothiri (Reg. No. MS14122)** for the partial fulfillment of BS-MS dual degree programme 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 25, 2019

Declaration

The work presented in this dissertation has been carried out by me with 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.

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

Dr. Abhishek Chaudhuri
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Dedicated to all my friends and family

Abstract

In this work, we study the phase separation of brownian particles driven by activity. These particles which are self propelled with the direction of motion relaxing through rotational diffusion. As in [\[Redner 13\]](#) we first show that the suspension of ABPs, modelled as discs, can cluster even in the absence of an attractive interaction. Next, as in [\[Stenhammar 15\]](#) we look at binary mixture of active and passive particles and show activity induced phase separation of two. We look at the orientational order parameter to understand the structural properties of the clustered state.

Chapter 1

Introduction

The story of life on earth has started roughly about 4.28 billion years ago. The widely accepted hypothesis regarding the origin of life is abiogenesis where life originates gradually from non living matters. This hypothesis was experimentally demonstrated by Miller and Urey in 1953 [Miller 53]. The transformation from such a unicellular prokaryote to the present multicellular eukaryotic organism – comprising of sophisticated organizational structure at every minute level– is intriguing. Today life has evolved into a broad spectrum spanning millions of different species each coexisting peacefully, and their interactions with abiotic components collectively gives shape to nature. Trying to understand the physical principles which govern life is a challenging problem and indeed a highly complex one.

1.1 Active Matter

There has been a lot of recent work which have tried to give a statistical description of living systems. These systems are now classed as “active matter”. This is a purely interdisciplinary field which incorporates experimental techniques from biology and chemistry along with simulations and theoretical approaches from physics to develop a proper understanding of the underlying phenomenon. The out of equilibrium behavior of individual units such as the movement of birds, animals or micro organisms, or

synthetic self-propelled particles, or the collective dynamics of these individual units interacting with each other are a few examples of such systems. The prospects of understanding the dynamics of living systems and using the knowledge to transport drugs to specific regions in the body or designing smart devices and materials, to name a few possibilities, makes it a fascinating field of research.

1.1.1 Individual dynamics

Active systems comprise of a large number of self driven units, each capable of converting either self stored or ambient free energy into systematic movement [Marchetti 13]. These self driven units vary from microscopic (migrating bacterial cells, actin-myosin mesh under plasma membrane, asters formed by microtubules, cytoskeletal filaments and motor proteins) to macroscopic (school of fishes, flock of birds, herd of horses) in terms of length scales (figure 1.1). One of the key ingredients of the dynamics of these individual units is the random behavior which is known as Brownian motion. The equilibrium statistical theory of Brownian motion describes a diffusive behavior characterized by a linear dependence on time of the mean squared displacement of the particle at long times. We will review the details of Brownian motion in a later section. The theory of Brownian motion has been modified to describe the motion of biological agents which typically show larger diffusivity as compared to that in equilibrium. The description of active particles have to be augmented with the idea of self propulsion which needs to be incorporated in the dynamics.

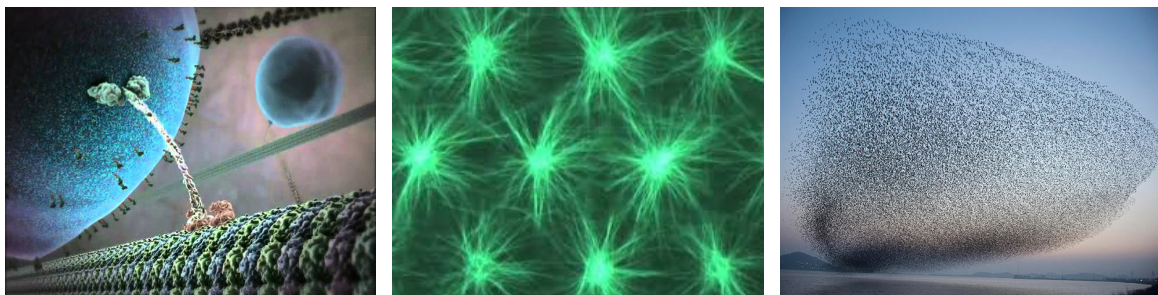


FIGURE 1.1: Left:- A motor protein carrying a vesicle through cytoskeletal filament inside a cell, Middle:- Asters formed in a suspension of microtubules on a cover slide, Right:-flock of birds

1.1.2 Collective dynamics

These living systems exhibit interesting emergent behaviours by collective self reorganization of individual units. Intricate dynamics of flocks of birds in flight, elegant maneuvers exhibited by school of swimming fishes, transport of vesicles by motor proteins through cytoskeletal filaments within a cell are few examples of such systematic movement exhibited by living systems [Menon 10]. This collective motion benefits the individuals of the system in several ways. Migratory birds take advantage of flocking dynamics to reduce the energy cost of the day long flight [Flack 18]. Within the flock itself assymetry can give rise to emergence of leadership and formation of subgroups [Ferdinandy 17].

One of the most important and early models of collective behavior of active matter was given by Vicsek et. al.[Vicsek 95]. They introduced a minimal model in which particles are driven with a constant velocity in random self propulsion directions. The movement of an individual unit proceeds in the average direction of motion of neighbouring units lying within a certain radius from it, with a small perturbation added to this average direction. This model showed the emergence of collective motion by spontaneous breaking of rotational symmetry.

1.2 Brownian motion

Brownian motion refers to the random jittery motion exhibited by small particles suspended in a fluid. The first experimental observation of this motion was done by Scottish Botanist Robert Brown [Brown 28] in 1827. He observed the motion of pollen grains suspended in water using a simple microscope. However, Brown was unable to give a scientific explanation of the origin of motion. In 1905, Albert Einstein provided a theoretical foundation of Brownian motion [Einstein 05]. The phenomenological approach of Brownian motion considers the process to be a stochastic process and constructs equations based on it. In this chapter we introduce and discuss Smoluchowski Equation and Langevin equation which describes Brownian motion.

1.3 Smoluchowski Equation

Consider a diffusion in one dimension. Let $c(x, t)$ be the concentration at x and t . Fick's law which provides the phenomenological description of diffusion process says, if there is a non uniformity in the concentration of particles, there will be a flux which is proportional to the concentration gradient.

$$J(x, t) = -D \frac{\partial c(x, t)}{\partial x} \quad (1.1)$$

where J is the flux and D the diffusion constant which depends on the temperature and size of the particle,

$$D = \frac{k_B T}{\zeta} \quad (1.2)$$

where k_B is Boltzmann constant, T is temperature and ζ is friction constant. The equation(1.2) is known as Einstein's relation. For a spherical particle of radius a , ζ is given by,

$$\zeta = 6\pi\eta a \quad (1.3)$$

where η is the coefficient of viscosity. Since the particle numbers are conserved, $c(x, t)$ should obey they continuity equation

$$\frac{\partial c(x, t)}{\partial t} = -\frac{\partial J(x, t)}{\partial x} \quad (1.4)$$

Combining equations (1.1) and (1.4) gives

$$\frac{\partial c(x, t)}{\partial t} = D \frac{\partial^2 c(x, t)}{\partial x^2} \quad (1.5)$$

Solving, $c(x, t)$ should has the functional form

$$c(x, t) = \frac{N}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \quad (1.6)$$

The mean squared displacement of the particle is given by,

$$\langle X(t)^2 \rangle = 2Dt \quad (1.7)$$

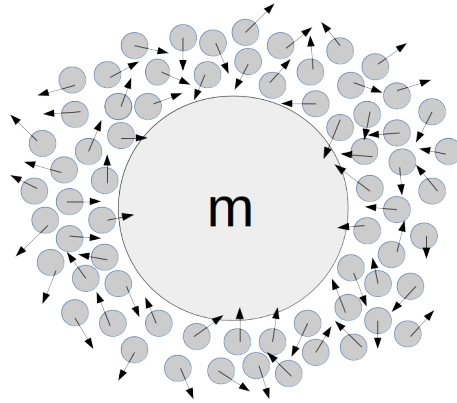


FIGURE 1.2: Brownian particle of mass m surrounded by fluid particles

Thus the particle concentration should spread out uniformly and it should be proportional to the square root of time.

In the presence of an external potential $U(x, t)$, the particles will experience a force,

$$F = -\frac{\partial U(x)}{\partial x} \quad (1.8)$$

and thus the diffusion equation modifies to

$$\frac{\partial c(x, t)}{\partial t} = \frac{\partial}{\partial x} \frac{1}{\zeta} \left(k_B T \frac{\partial c}{\partial x} + c \frac{\partial U}{\partial x} \right) \quad (1.9)$$

Equation (1.9) is known as Smoluchowski equation [Doi 88].

1.4 Langevin Equation

Consider a Brownian particle of mass m immersed in a fluid of viscosity η as shown in figure 2.1. The Newton's equation of motion governing the motion of the Brownian

particle in one dimenaion is,

$$m \frac{dv}{dt} = F_{total}(t) \quad (1.10)$$

Since we know that the major contribution is from the viscous force exerted by the fluid, equation (1.10) can be written as,

$$m \frac{dv}{dt} = -\zeta v \quad (1.11)$$

where ζ is the friction constant and v , the velocity of the particle. Solving the above differential equation(1.11) will give

$$v(t) = v(0)e^{\left(\frac{-\zeta t}{m}\right)} \quad (1.12)$$

Thus based on the equation (1.12) the velocity of the particle should decay to zero in longer times. This is in contradiction with the fact that the mean squared velocity of the particle in thermal equilibrium should be $\frac{k_B T}{m}$. Hence the assumption of F_{total} being dominated by friction alone needs to be scrutinized.

At each instant the Brownian particle is colliding with a large number of particles in the surrounding fluid. The number of collisions and force exerted by these particles varies rapidly and we cannot quantify them. One way of tackling this would be to modify the equation (1.11) with a random noise term which accounts for the rapid collisions imparted by the surrounding fluid particles. Thus equation(1.11) becomes,

$$m \frac{dv}{dt} = -\zeta v + \delta F(t) \quad (1.13)$$

were $\delta F(t)$ is Gaussian white noise with

$$\langle \delta F(t) \rangle = 0 \quad (1.14)$$

$$\langle \delta F(t) \delta F(t') \rangle = 2B \delta(t - t') \quad (1.15)$$

Equations (1.14) and (1.15) sum up the properties of the fluctuating force. The delta correlated noise says there is no correlation between the noise at two instants t and t' . Here B determines the strength of the fluctuating force.

Equation (1.13) is called Langevin equation, which on solving yields

$$v(t) = e^{-\frac{\zeta t}{m}} v(0) + \int_0^t dt' e^{-\frac{\zeta(t-t')}{m}} \frac{\delta F(t')}{m} \quad (1.16)$$

Calculating mean squared velocity using (1.15) yields

$$\langle v(t)^2 \rangle = e^{-\frac{2\zeta t}{m}} v(0)^2 + \frac{B}{\zeta m} (1 - e^{-\frac{2\zeta t}{m}}) \quad (1.17)$$

The exponentials in the above equation (1.17) drops out in long time and hence approached $\frac{B}{\zeta m}$. Combining this with the equilibrium value $\frac{K_B T}{m}$ yeilds,

$$B = \zeta K_B T \quad (1.18)$$

The above obtained result (1.18) is known as fluctuation dissipation theorem. This relates the strength of fluctuating force and the friction coefficient or dissipation. In other words the balance between the fluctuations which keeps the system alive and dissipation which let the system die out[Zwanzig 01].

In the presence of an external force F , Langevin equation (1.13) modifies to

$$m \frac{dv}{dt} = F - \zeta v + \delta F(t) \quad (1.19)$$

1.5 Colloidal Systems

The Brownian motion of particles is difficult to observe. Colloidal systems which are micron sized particles suspended in liquids are an ideal system for observation and characterization. Colloids form an important part of our lives from food items to medicine. Colloidal system are excellent model systems for statistical physics. With the recent advances in the field of synthetic active matter, it is useful to divide colloidal systems into two parts : (i) Passive colloids and (ii) Active colloids.

1.5.1 Passive Colloids

As obtained in the previous section, the time scales for a colloid of micron size to diffuse over a length scale similar to its size would take seconds. This is a considerably large time scale to observe the dynamics of such systems as opposed to atomic systems. Further, the pairwise interaction of passive colloids can be easily tuned. This makes them ideal systems to study using computer simulations. Indeed a plethora of studies have revealed several interesting static and dynamic collective behavior of passive colloids.

1.5.2 Active Colloids

Active colloids on the other hand are far from equilibrium systems. Active colloidal suspensions consist of self propelling particles moving in a viscous fluid either by consuming self generated energy or by extracting the energy from ambient environment. One of the key features of such colloidal suspensions is that they exhibit dynamic self assembly, forming structures like the plasma membrane of a living cell. Such features make active colloidal suspensions a good starting point to model active systems.

1.6 Plan of the Thesis

In this thesis, we first look at a colloidal system of soft discs in two dimensions, which are self propelled. As in [Redner 13] we look at the effect of activity on the collective dynamics of these particles. Then we look at a mixture of active and passive discs and look at the effect of activity on clustering in this system.

Chapter 2

Phase Separation in Active Colloids

In this chapter we look in to a colloidal system in two dimensions comprising of self propelled particles interacting by an excluded volume interaction. In the first section a minimalistic theoretical discription of the model introduced by [\[Redner 13\]](#) is discussed. Later using molecular dynamics simulations, activity induced phase separation into a dense solid like phase is studied.

2.1 Model Description - Self Propelled Particles

The system comprises of a large number of self propelled smooth discs immersed in a fluid of viscosity η confined in a two dimensional plane. The particles interacts each other by purely repulsive Weeks-Chandler-Anderson (WCA) potential. The N particle system is completely specified by the positions (r_i) and self propulsion directions (θ_i) of the particles. The system evolves in time with the following overdamped Langevin equation

$$\dot{\mathbf{r}}_i = D\beta[\mathbf{F}_{ex}(r_i) + \mathbf{F}_p\hat{\mathbf{v}}_i] + \sqrt{2D}\boldsymbol{\eta}_i^T \quad (2.1)$$

$$\dot{\theta}_i = \sqrt{2D_r}\eta_i^R \quad (2.2)$$

where, $F_{ex}(r) = -\frac{dU_{ex}(r)}{dr}$, is the repulsive force due to the WCA potential, $U_{ex}(r)$.

$U_{ex}(r)$ is given by,

$$U_{ex}(r) = \begin{cases} 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right] + \epsilon & \text{if } r < 2^{\frac{1}{6}}\sigma \\ 0 & \text{otherwise} \end{cases} \quad (2.3)$$

which prevents the particles from overlapping. Here, σ is particle diameter and $\epsilon \equiv k_B T$ is the strength of the potential. D and D_r are translational and rotational diffusion constants respectively. In the low Reynolds number limit, they are related as

$$D_r = \frac{3D}{\sigma^2} \quad (2.4)$$

The self propulsive force which moves each particle with speed $v_p = D\beta F_p$, drive the system out of equilibrium. The direction of the particle is specified by $\hat{\mathbf{v}}_i = (\cos\theta_i, \sin\theta_i)$. Here $\beta = \frac{1}{k_B T}$ and η^T, η^R are uncorrelated Gaussian noise with

$$\langle \eta \rangle = 0 \text{ and } \langle \eta_i(t)\eta_j(t') \rangle = 2D\delta_{ij}\delta(t-t') \quad (2.5)$$

The density of the particles is set by $\rho = \frac{N}{L^2}$. The active drive is controlled by the dimensionless Peclet number, $Pe = \frac{v_p\tau}{\sigma}$. This is the ratio of advection to diffusion at the scale of particle size. Here τ is translational relaxation time.

2.2 MD Simulation

We used σ , $k_B T$ and $(\tau = \frac{\sigma^2}{D})$ as basic units of length, energy and time scales respectively. These are used to make the equations of motion(2.1) and (2.2) dimensionless. Simulations were carried out by numerically integrating the equations of motion ((2.1) and (2.2)) using stochastic Runge-Kutta method [Brańka 99]. The system comprises of (N=2500) particles arranged homogeneously ($\rho = 0.7$) in a square box with

periodic boundary conditions and random self propulsion directions. In each time step the total force on each particle is calculated and the particle positions are updated accordingly. First 10^6 time steps were left for the system to reach steady state and particle configurations were analyzed at constant intervals in the next 10^6 time steps. The most time consuming part in the simulation is the force calculation which scales as N^2 where N is the number of particles. In order to reduce this, we parallelized the force calculation by threading the loops using OPENMP.

2.3 Phase Separation

To understand the dynamics of the system, we calculate the local density distribution and look at the variation of with change in activity. From the particle configurations and the local density distribution, we observe that the particles are homogeneously distributed as a single phase with local density distribution peaked around $\rho = 0.7$ which is the equilibrium density of the system. Increasing peclet number to $Pe = 50$, we observe that the system still remains in single phase but the local density distribution spreads showing the formation of small clusters due to the increase in activity. Further increasing peclet to $Pe = 90$, the local density distribution becomes bi-modal with one peak around 1.3 corresponding to a dense clustered phase and the other one around 0.4 corresponding to homogeneous liquid phase. Finally for $Pe = 150$, the peaks spreads more corresponding to increased density of clustered phase (peaked around 1.5) and the less dense liquid phase (peaked around 0.4). Even when there are no attractive interaction between the particles, the system exhibits non equilibrium clustering similar to the equilibrium phase separation in presence of attractive interaction seen in passive systems. System goes from a homogeneous liquid phase to a solid-liquid coexisting phase as we increase the control parameter Pe which accounts for the activity.

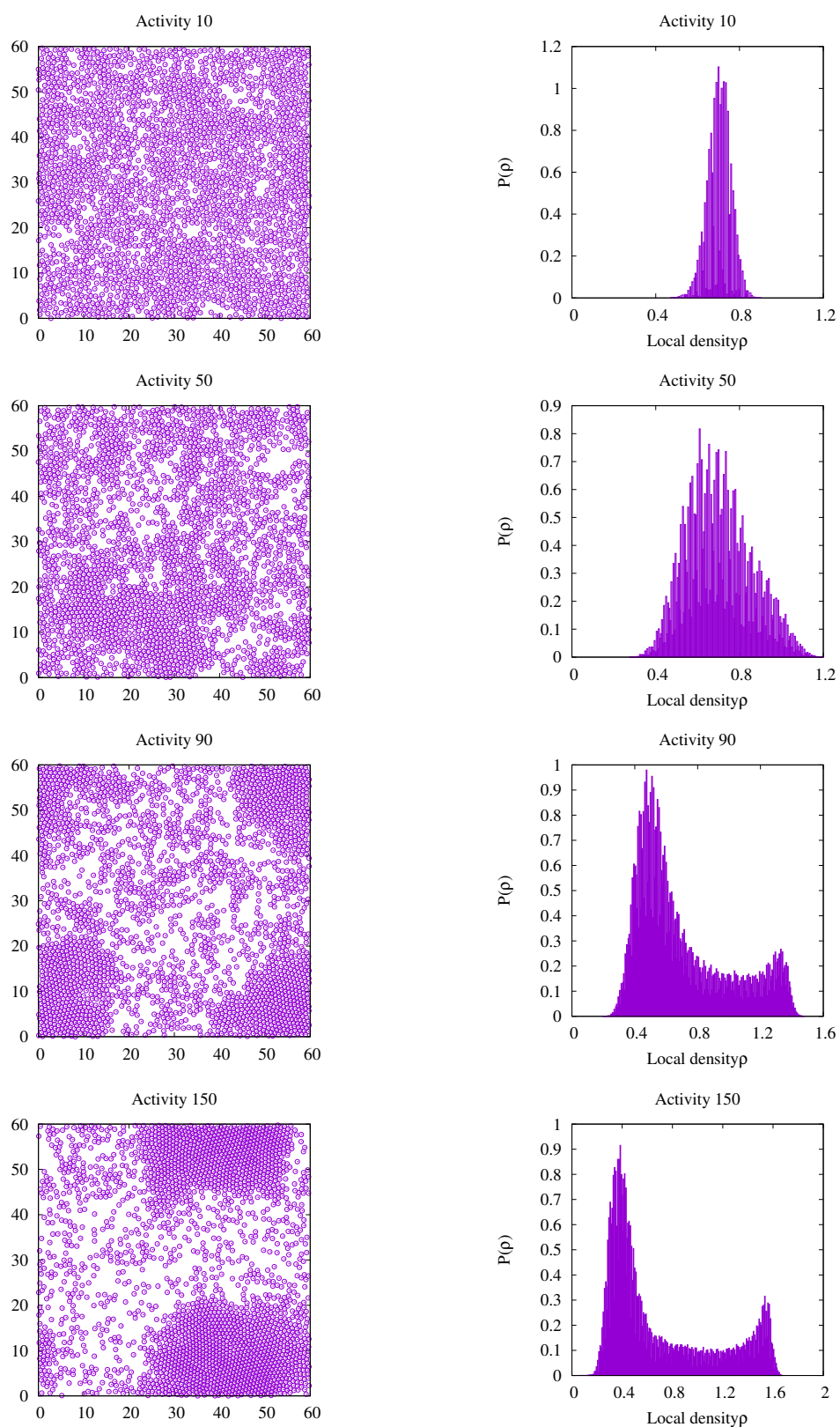


FIGURE 2.1: Left:- Snapshots of the system after reaching steady state for different Peclet numbers(10, 50, 90, 150) , Right:- Local density distribution for different Peclet numbers

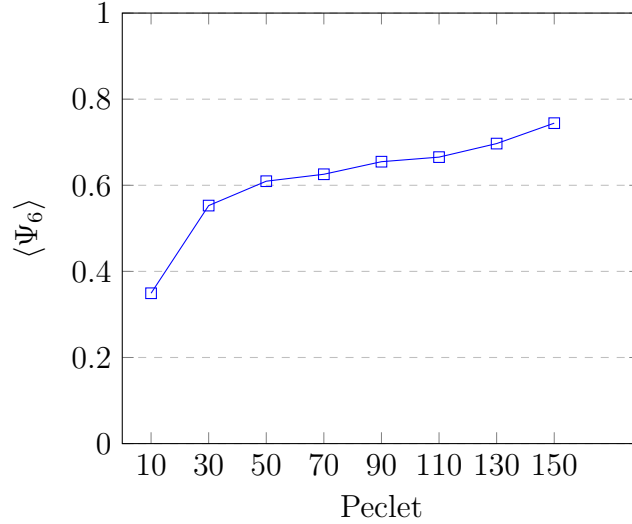


FIGURE 2.2: Variation of bond orientation order parameter Ψ_6 with Pe .

2.3.1 Bond Orientation Order Parameter

To characterize the system further, we look at structural properties of the system, using bond orientational order parameter. To understand what it means, consider a periodic crystal in which particles are fixed on a lattice. In such a crystal, one can specify the position of nearest neighbours using a discrete set of directions defined by the vectors between the position of neighbours. This set of direction is universal throughout the crystal giving rise to a long range order which is often known as bond orientation order. The local orientational order of a particle located at a position $\mathbf{r}_i = (\mathbf{x}_i, \mathbf{y}_i)$ can be specified by a local value of bond orientational order parameter which is defined as

$$\Psi_{6,i} = \frac{1}{N_b} \sum_{j=1}^{j=N_b} \exp(i6\theta_{ij}) \quad (2.6)$$

where N_b is the number of neighbouring particles and θ_{ij} is the angle made by the inter-particle vector of particles i and j and a fixed axis [Mazars 08]. A global bond orientational order parameter can be calculated by taking an ensemble average of the local bond orientational order parameter (2.6).

$$\langle \Psi_6 \rangle = \left\langle \frac{1}{N} \sum_{i=1}^{i=N} |\Psi_{6,i}| \right\rangle \quad (2.7)$$

where N is the total number of particles in the system. In figure 2.2 we show the

variation of $\langle \Psi_6 \rangle$ as the activity is increased. For lower Pe , the system shows liquid like behaviour with a very small orientational order parameter value. As the activity is increased, there are large regions of clustered phase which leads to a high $\langle \Psi_6 \rangle$, indicative of a hexatic ordering in the system.

2.4 What Gives Rise to Clustering?

To answer this question, we follow the argument given in [Cates 13]. Let us consider a suspension of active particles. In the presence of concentration gradient, the flux of the particles is given by Fick's law as ,

$$\vec{J} = -D\vec{\nabla}\rho \quad (2.8)$$

where D is the diffusion constant. If D is spatially uniform, the system relaxes to a homogeneous state given by $\vec{\nabla}\rho = 0$. If however D is space dependant, then the flux is modified to

$$\vec{J} = -D(\mathbf{r})\vec{\nabla}\rho - k\rho v(\mathbf{r})\vec{\nabla}v \quad (2.9)$$

where k is a constant depending on dimensionality and the frequency of rotational relaxation events. For interacting particles, the speed of the particles depends on the local density of the particles, ie:- $v(\mathbf{r}) = v(\rho(\mathbf{r}))$. Thus equation (2.9) becomes

$$\begin{aligned} \vec{J} &= -\left[D(\rho) + k\rho v(\rho)\frac{dv}{d\rho}\right]\vec{\nabla}\rho \\ &= D'(\rho)\vec{\nabla}\rho \end{aligned}$$

and

$$\frac{\partial\rho}{\partial t} = -\vec{\nabla}\vec{J} = \vec{\nabla}\cdot(D'(\rho)\vec{\nabla}\rho)$$

Thus the speed of particles can change steeply with density and then $D'(\rho)$ can become negative which can lead to non-uniform steady states. This is the idea of motility induced phase separation (MIPS) where a local density fluctuation can lead to particle

slowing down which acts as a feedback and can lead to more particles accumulating, giving rise to a large cluster.

Chapter 3

Binary Mixture of Active and Passive Colloids

In the previous chapter, we considered the case of active particles of one type. The natural question to ask is what will happen when we have two types of particles with different motility or size. To answer this we looked at a binary mixture of active and passive particles. By passive we mean that they are non motile. This part of thesis is based on the paper by Stehnammar et al.. [[Stenhammar 15](#)]. The first section deals with the modifications made in the model from the one discussed in Chapter 2. In the consequent sections, we discuss the activity induced phase separation and the phase behaviour.

3.1 Model Description

The system comprises of active particles whose time evolution is given by over damped Langevin equations (2.1) and (2.2). The passive particles in the system time evolves based on Langevin equation (2.1) with $F_p = 0$. Despite from directly increasing the swim speed, here we employ a different implementation for increasing the activity of the system [[Stenhammar 14](#)] which is detailed below.

3.1.1 Variation of Peclet

In the previous chapter when we looked into purely active systems, we used F_p as a free parameter to vary Peclet. Looking from an energy perspective Pe is the ratio between the ballistic energy $F_p\sigma$ and the thermal energy $k_B T$. These two are the only kinds of energy scale in the case of hard spheres and hence Pe can uniquely determine the balance between the two. However the particles in our systems are not infinite hard spheres and a new energy scale arises from the steepness of the WCA potential which is controlled by ϵ . Thus ratio $\epsilon/k_B T$ which specifies the hardness of the particles also come into picture and Pe alone will not be sufficient to describe the system [Stenhammar 15]. In Chapter 3, we fixed $\epsilon/k_B T = 1$ and varied F_p directly. But in this case $\frac{F_p\sigma}{\epsilon}$ is no longer constant and at higher Pe this can lead to increased overlap between the particles which can lead to non physical scenarios. In order to overcome this hurdle we keep the active force at a constant value $F_p = \frac{24\epsilon}{\sigma}$ and vary the rotational diffusion time scale to vary Pe .

$$Pe \equiv \frac{3v_0\tau_r}{\sigma} \quad (3.1)$$

Equation (3.1) is in accordance with the definition in chapter 2. Thus a higher Pe value leads to a small D_r , and hence rather than exerting more force on the self propulsion direction, a constant force is being applied to the self propulsion direction for an increased time.

3.2 MD Simulation

Simulations were started by switching on active force F_p using a quench from equilibrated passive colloidal configurations. The system comprised of 2500 brownian particles in a square box with periodic boundaries and overall density ($\rho = 0.6$). Out of the 2500 particles, X_a fraction of particles were active while the remaining were passive. Total forces acting on each particles were calculated at each time step and

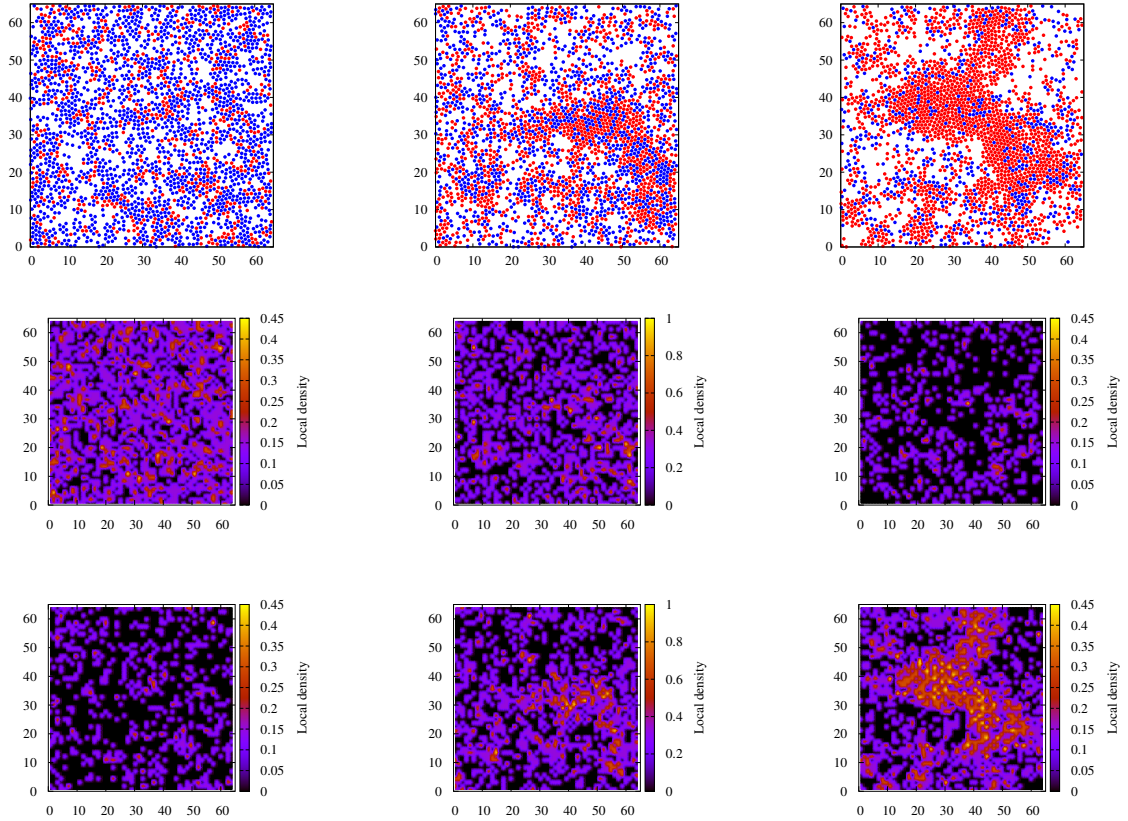


FIGURE 3.1: Top:- Snapshots of particle configurations $X_a = 0.25, 0.5, 0.75$ respectively, Middle:- Surface density plot of passive particles $X_a = 0.25, 0.5, 0.75$ respectively, Bottom:- Surface density plot of active particles $X_a = 0.25, 0.5, 0.75$ respectively, $\rho = 0.6, Pe = 300$

positions were updated accordingly. First 4×10^7 time steps were left for the system to reach steady state and the next 10^7 particle configurations were analyzed at regular intervals.

3.3 Phase Separation

We look at the local density plots of both active and passive particles and system configurations of these particles. The system remains homogeneous for lower active particle fraction (X_a). The first column of figure 3.1 depicts the particle configuration as well as local density of active and passive particles of a system with active particle fraction ($X_a=0.25$). Increasing the active particle fraction X_a to 0.5 results in the formation of clusters. An interesting observation here is that the spatial distribution

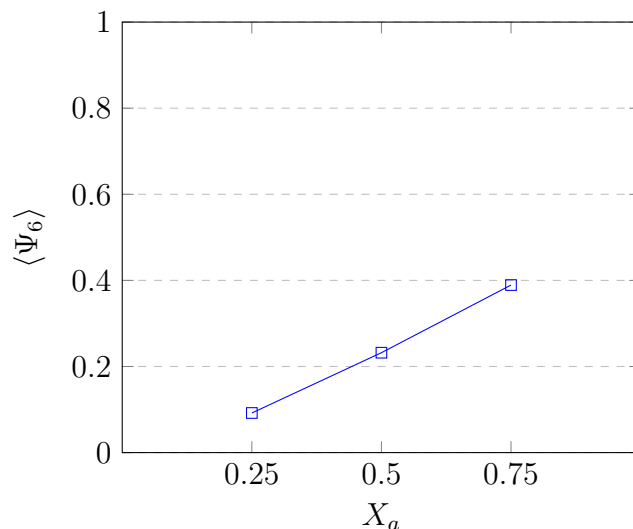
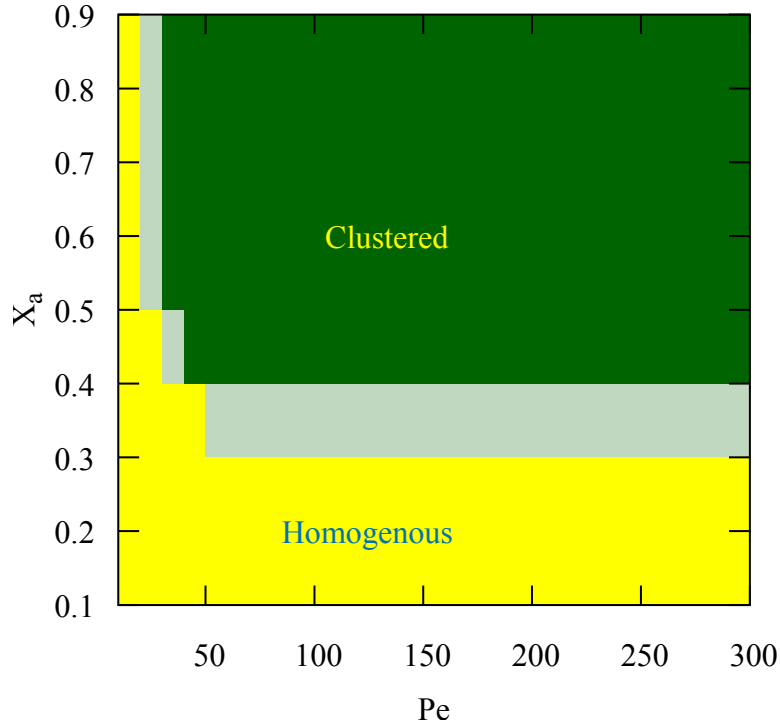


FIGURE 3.2: Variation of bond orientation order parameter Ψ_6 with X_a ($Pe = 300$, $\rho = 0.6$)

of active and passive particles are not homogeneous. Passive particles are mostly concentrated inside the cluster whereas active particles are distributed towards the periphery. Within the cluster, small clusters of passive particles can also be observed (second column of figure 3.1). Further increasing the active particle fraction X_a to 0.75, the clustering increases and becomes more dense (third column of figure 3.1).

Then, there is a spontaneous segregation of active and passive particles although the segregation is naturally different from that observed in passive binary mixtures. This segregation is induced by the activity. Further, unlike the situation of single active particle suspension showing MIPS, here the clusters constantly move and break up and fuse. In the single particle case, the cluster once formed is mostly stationary although there are fluctuations. The bond orientational order parameter (figure:-3.3) shows an increase as the active particle fraction is increased at a given Pe . This is expected since the clustering and segregation becomes more pronounced at higher activity.

FIGURE 3.3: Phase diagram in $X_a - Pe$ plane.

3.4 Phase Behaviour

In the phase diagram in $Pe - X_a$ plane (figure 3.3), we see spontaneous separation of phases for small particle fractions ($X_a \equiv 0.3$) as well. This happens at higher Pe . For very small Pe , phase separation is not observed even for higher active particle fractions. The phase boundary is supposed to follow a functional form, ($X_a \sim \frac{1}{Pe}$) [Stenhammar 14]. However due to the smaller number of particles considered in this simulation, we do not observe the same behaviour.

Chapter 4

Summary

In this work, we started with a minimal model describing the active self propelling particles in two dimensions. Using molecular dynamics (Langevin dynamics), we showed that the system comprising of particles interacting with purely repulsive interactions exhibit activity induced clustering which eventually facilitates a solid-liquid phase separation. We have looked at the structural properties of dense phase by calculating the bond orientation order parameter and showed that dense cluster approaches hexagonal packing. In the second part of the work, we introduced passive particles into system and looked at the structural and phase behaviour by varying active particle fraction X_a and Pe . An interesting finding is that the spatial distribution of active and passive particles are not homogeneous within cluster. Passive particles are located towards the interior of the clusters while active particle are concentrated towards the periphery. While exploring the phase behaviour in $X_a - Pe$ plane, we showed that the system still exhibits phase separation above a threshold activity and X_a .

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