Chapter 1

Introduction

1.1 Statistical mechanics and its development

In Statistical Mechanics, we tried to explore probability theory and statistics. Statistical mechanics combines the principles and procedures of statistics with the laws of both classical and quantum mechanics, particularly with respect to the field of thermodynamics. It aims to predict and explain the measurable properties of macroscopic systems based on the properties and behavior of the microscopic constituent of those systems. Statistical mechanics was started around the 1870s with the benchmark work of Boltzmann [Boltzmann (1964); Fowler (1967); Huang (1987, 2008); Uffink (2017)]. Boltzmann's study on the statistical interpretation of thermodynamics, the H-theorem, transport theory, thermal equilibrium, the equation of state of gases, etc. Boltzmann introduced the notion of an equilibrium statistical ensemble and also tried to investigate, for the first time, nonequilibrium statistical mechanics, with the help of the H-theorem [Huang (1987); Pathria (1996); Uffink (2017)]. Other researcher like Clerk Maxwell [Grant & Phillips (2013); Maxwell (1995)], Josiah Willard Gibbs [Klein (1990)], and Albert Einstein [Foley (1951); Sen (2021)] play eminent participation in the formulation of this area. A mathematical framework is defined in terms of a more detailed analysis, like the dynamics of individual particles. Later on, the laws

of thermodynamics are formulated in a more profound theory by applying statistical mechanics [Hill (2013); Pathria (1996); Zemansky & Dittman (1997)]. Statistical mechanics does not tell us about the details of the individual particle's motions. Instead of that, they collectively behave like a continuous fluid. That is the basic intuition about statistical mechanics, which gives the exact probabilistic insight of high-level description and averaging of lots of systems and appropriate pieces of information. Hitherto, we agree that statistical mechanics accounts for the deeper degrees of freedom and aims to connect the macroscopic and microscopic properties of matter in thermodynamic equilibrium [Fowler (1967); Huang (2008); Pathria (1996); Zemansky & Dittman (1997)] which provides the physical properties of the matter on different time and length scales by calculating the statistical fluctuations [Huang (1987); Pathria (1996); Zemansky & Dittman (1997)].

Now we will make the connection between thermodynamics and statistical mechanics. In statistical mechanics, we formulate the problem in different ensembles [Huang (2008); Maxwell (1995); Pathria (1996); Zemansky & Dittman (1997)] (i) Microcanonical (N,E,V): where total number of particles in the system (symbol:N), the system's volume (symbol: V), as well as the total energy in the system (symbol: E). Each of these quantities is assumed to be constant in this ensemble. Because of that, the microcanonical ensemble is known as N,V,E ensemble. (ii) Canonical (T,V,N): where T is absolute temperature (symbol: T) of the medium, the number of particles in the system (symbol: N) and the system's volume (symbol: V), remain constant. Hence the canonical ensemble is also known as N,V,T ensemble and (iii) Grand canonical ensemble (T,V,μ): where chemical potential (symbol: μ), absolute temperature (symbol: T) and volume (symbol: V) this ensemble is known as T,V,μ ensemble.

Considering a system of N identical particles in a volume V and energy E, the macrostate of the system is defined by variable (N,E,V). Additionally, there are many ways in which the total energy of the system E is distributed among the N particles. Since there are vari-

ous possible arrangements of the particles, which are known as microstates of the system [Fowler (1967); Pathria (1996); Zemansky & Dittman (1997)]. Therefore, to describe the system in three-dimensional space $(3D)$, a total $6N$ degrees of freedom are required to construct the phase space. Each point (which will have $3N$ coordinates and $3N$ momenta) represents configuration of particles in the phase space. Which is termed as a microstate of the system. In contrast, the collection of a large number of such microstates is known as a macrostate of the system. When we start observing the system we sample (average) over large number of microstates of a given macrostate of the system. The averaging is performed based on the postulates of equilibrium statistical mechanics:

(i) A priori Probability: it refers to the likelihood of an event occurring when there is a finite number of outcomes, and each outcome is equally likely to occur.

(ii) Ergodic Hypothesis: The time spent by a system in some region of the phase space of a microstate with the same energy in equivalent to the volume of the region.

3) Boltzmann's hypothesis: A trajectory explored by the particle in the hypervolume ω in the phase space, then the entropy of the system is defined as $s = k \ln \omega$, where k is Boltzmann's constant [Pathria (1996); Uffink (2017); Zemansky & Dittman (1997)]. Boltzmann's relation provides the bridge between statistical mechanics and thermodynamics. Till now we have discussed the concepts of statistical mechanics for systems in thermal equilibrium. But most of the natural systems are nonequilibrium; Their examples range from: protein folding and unfolding, fish schools [Katz et al. (2011)], bird flocks [Ballerini et al. (2008)], molecular machines, actin filaments [Hubbard et al. (2004)], microtubules, motile cells [Sumino et al. (2012)], colloidal rollers [Morin et al. (2017)] and autophoretic colloids [Buttinoni et al. (2013); Palacci et al. (2013); Theurkauff et al. (2012)], glassy state, rheology of biological suspension [Giomi et al. (2010); Hatwalne et al. (2004); Liverpool & Marchetti (2006)], turbulence, time-dependent Hamiltonian systems [Struckmeier & Riedel (2001)], driven systems etc.

Understanding of the nonequilibrium systems in the framework of statistical mechanics is an emerging area. Recently researchers are paying ample attention to understand the properties of nonequilibrium systems. Nowadays, a whole class of biological and physical systems are referred to active matter, studied theoretically and experimentally. These systems are in general nonequilibrium [Bendix et al. (2008); Dombrowski et al. (2004); Peruani et al. (2012); Rafaï et al. (2010); Sumino et al. (2012); Szabó et al. (2006)]. The term "active" referrers to the ability of individual particles to move by gaining energy from their surroundings [Cates (2012); Marchetti et al. (2013); Ramaswamy (2017); Toner et al. (2005); Vicsek & Zafeiris (2012); Yates et al. (2010)]. Due to the dynamics on each particle level, dynamics of such system breaks the time reversal symmetry. Hence, in general the transition from one state to other state of these systems does not satisfy the principle of detailed balance, which is a basic feature of any equilibrium system. Next we discuss the principle of detailed balance.

Principle of detailed balance:-

The detailed balance principle was first developed by Boltzmann [Boltzmann (1964)] based on the time reversal symmetry of the states in an equilibrium system. When a system goes from state 1 to state 2, from state 2 to state 3 and then from state 3 to state 1, there is no net flow of probability in an equilibrium system. Whereas in a nonequilibrium system there is a net flow of probability for going from one state to another hence in general detail balance is violated. The schematic of the detail balance condition in an equilibrium systems shown in Fig. 1.1. Using π_i as the probability of being in state i and q_{ij} is the transition probability from state i to state j, then $\pi_i q_{ij}$ shows the "amount" of current that flows down the edges $i \to j$. If detailed balance condition is satisfied as shown in Fig. 1.1. The current flowing from i to j, equals the amount that flows from j to i. Hence, there is no net flux along the edge $i \leftrightarrow j$, provided the chain is in the stationary distribution. Same condition is shown by Kolmogorov's condition [Kolmogoroff (1936)] using probability $P(i, j)$ as the

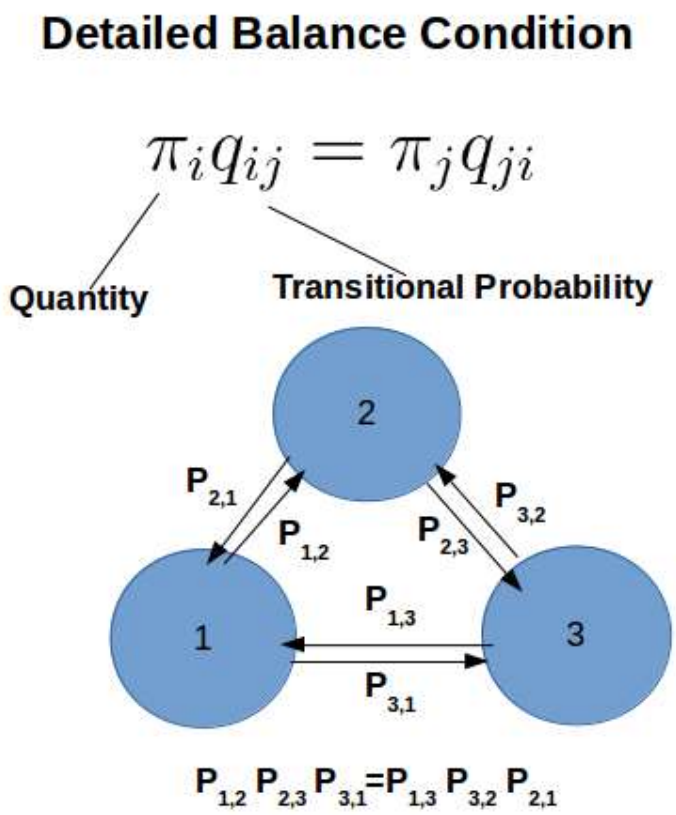

Fig. 1.1 Schematic diagram of detailed balance condition(top). (bottom): Shows the Kolmogorov's condition for detail balance.

transition probability from state i to state j. Now we discuss the basic properties of active matter systems in following section.

1.2 Active matter system

Active matter is composed of active particles: these active particles have the ability to gain energy from the environment, like an internal fuel tank, and convert this energy into the motion of an internal motor coordinate along the direction of asymmetry of the particle [Cates (2012); Marchetti et al. (2013); Ramaswamy (2010, 2017); Toner et al. (2005); Vicsek & Zafeiris (2012); Yates et al. (2010)]. It makes the particles self-propel with a

self-propulsion speed. And particles are referred as "self-propelled particles" (SPP) with a finite speed called as self-propulsion speed (SPS). The finite self-propulsion speed makes the system essentially nonequilibrium and many interesting phenomena like complex patterns in the sky birds flock [Cavagna & Giardina (2014)], fish schools [Katz et al. (2011)], etc. Biological examples of self-propelled particles are pretty abundant in natural systems. These are often quite complex: For example, the rich phenomenology of bacterial suspension in the combination of their self-propulsion speed, the alignment interaction because of their rod-like shapes, and the hydrodynamic coupling of the medium where they swarm [Sokolov et al. (2007)]. In this thesis, we will focus on the dynamics and kinetics [Nelson (2007); Tayler & group (2013)] of active particle systems.

All of the active systems outlined above, each SPPs advances at the expense of its internal energy, which is translated into mechanical motion. Because energy is supplied at each particle level, active systems are different from other nonequilibrium systems, such as a bulk fluid sheared from the top [Hemingway et al. (2016); Menzel (2015); Saracco et al. (2011); Saracco et al. (2012)] or diffusive system with some external drive [Balakrishnan (2021); Brangwynne et al. (2009); Garrido et al. (1998); Schmittmann & Zia (1991)]. In analogy with an equilibrium system which has a well defined steady state, a nonequilibrium system, is defined by a nonequilibrium steady state (NESS). In contrast to an equilibrium steady state which in general has non-zero current, a NESS is defined with non-vanishing fluxes in the system [Kirkpatrick et al. (1982); Lax (1960)] For example in a flock of birds, where all of the agents move in unison, can be describe as a NESS of the system.

Another interesting feature of active matter system, which is very specific to this class of nonequilibirum system is the large density fluctuations in the steady state. The density fluctuation in these systems is significantly greater than the usual equilibrium system. In an equilibrium system, density fluctuation is $\Delta N \propto \sqrt{N}$ provided the system is away from the critical point, where N is the number of particles in a finite volume V. Also it is

independent of dimensionality of the system. In an active system the density fluctuation is much larger than $\sqrt{N}$ and it depends on the demensionality of space. Specially in two-dimensions it can be as large as proportional to N for larger N [Ramaswamy et al. (2003)].

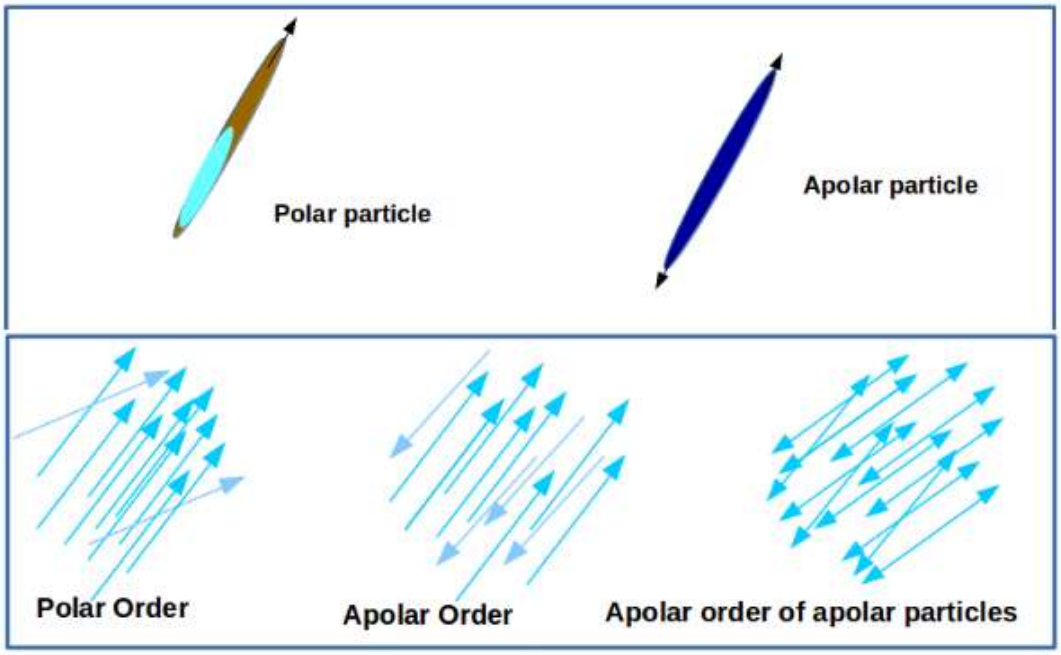

Fig. 1.2 Schematic diagram of different type of particles polar and apolar. Where arrows shows the direction of motion. Where bottom panel shows the different order corresponding to different particle.

1.2.1 Types of active particles

Based on the symmetry of the particles and shape and their nature of alignment we can distinguish them into different types of active particles. Broadly speaking we have two types of active particles: particle with head and tail symmetry called as apolar active particles and particles with different head and tail are called as polar particles. We further characterise them in following manner: whether they are asymmetric/symmetric in shape and can align or not with their neighbours.

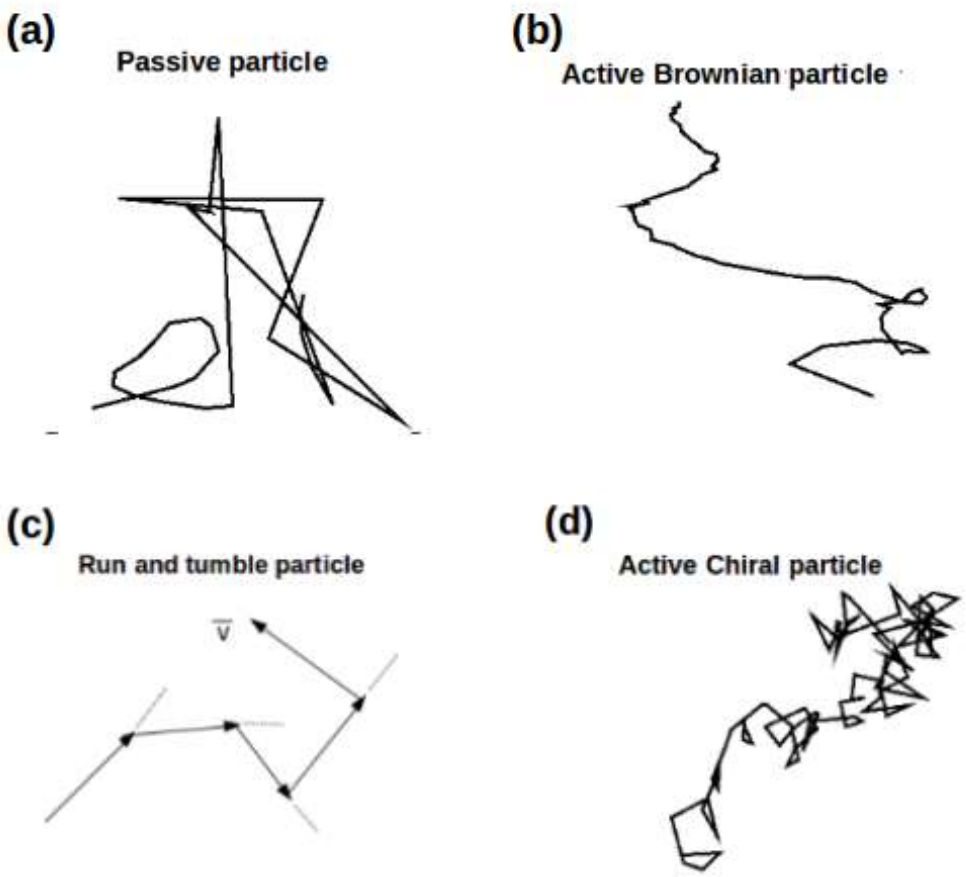

Fig. 1.3 Trajectories of (a) passive Brownian particle, (b) active Brownian particle (ABP), (c) Run and tumble particle(RTP), (d) active Chiral particle(ACP).

Polar particles with alignment interaction:- These particles have different head and tail symmetry and due to asymmetric body shape they can also align with their neighbours when comes in contact as shown in Fig.1.2. Examples range from small scales inside our cells: microtubules and cytoskeleton filaments [Marchetti et al. (2013); Needleman & Dogic (2017); Ramaswamy (2010)], bacterial suspension [Bär et al. (2020)], to large scale bird flock [Ramaswamy (2017)], fish school [Ramaswamy (2010)], animal herd [Shaebani et al. (2020)] and even the dead tapered copper rods [Kumar et al. (2019)]. Later, we discuss the microscopic rules for their dynamics when placed in collection.

Apolar particles with alignment interaction:- When particles cannot be distinguished

with head and tail, but possess an asymmetric body shape, such that they align either parallel or antiparallel with their neighbours are called apolar particles as shown in Fig.1.2. When placed in collection, they can align with their body axis parallel to each other and form an ordered state called as nematic state. Because of active nature of these particles, the nematic state have many interesting properties which are not present in general in their passive counterpart and they are called as active nematics. The examples of such systems are melanocyte cells [Fu et al. (2022); Marchetti et al. (2013); Ramaswamy (2010)], active motililty assays [Kierfeld et al. (2008)], dead vibrated copper rods [Kumar et al. (2019)], living liquid crystals etc.

Active Brownian particles:- Another class of particles, which are spherically symmetric in shape, such that they do not have alignment interaction but due to their self-propelled nature can move along one direction known as Active Brownian particle(ABP) as shown in Fig. 1.3(b). If self-propulsion is turned off the dynamics of such a particle is very much similar to passive Brownian particles as shown in Fig. 1.3(a). Due to the presence of activity they are named as Active Brownian particles (ABPs). Examples of such particles are many bacteria, which are nearly spherical in shape [Romanczuk et al. (2012); Solon et al. (2015)], or artificially designed active Janus particles [Choudhury et al. (2017); Semwal et al. (2021)], active colloids [Zhang et al. (2017)] etc. If the direction of self propulsion of these particles changes continuously then their trajectory is smooth and particles are referred as active Brownian particles (ABP). Whereas many bacteria like E-coli [Patteson et al. (2016)] move in a certain direction for sometime and then perform the random tumble event and hence such dynamics are called run and tumble dynamic and particles named as run and tumble (RTP) particles [Solon et al. (2015)] as shown in Fig.1.3(c). The steady state characteristics of both types of particles are same and one can be mapped to other [Shaebani et al. (2020); Solon et al. (2015)].

When placed in collection the ABPs show the phase separation at very small packing

fraction in comparison to their equilibrium counterpart. Such phase separation is solely due to motility of particles. Hence it is called as motility induced phase separation (MIPS) [Bechinger et al. (2016); Cates & Tailleur (2013, 2015); Shaebani et al. (2020)].

Most of the computational models of active particles assume particles have left and right symmetry and hence they swim in straight line. In reality, the left-right symmetry with respect to the internal propulsion direction must not be disturbed in order for optimal straight swimming to occur; even minor breaks in this symmetry causes any straight motion to become unstable and make them chiral, as shown in Fig.1.4. The motion of the particle is left, or right chiral depending upon which type of symmetry is broken. Such particles are called as active chiral particles (ACP) as shown in Fig. 1.4, 1.3(d). Jennings (1901) first noted the presence of microorganisms swimming in circles, and since then, it has been seen in a variety of settings, particularly adjacent to a substrate for bacteria [Huang et al. (2020); Ma & Ni (2022)].

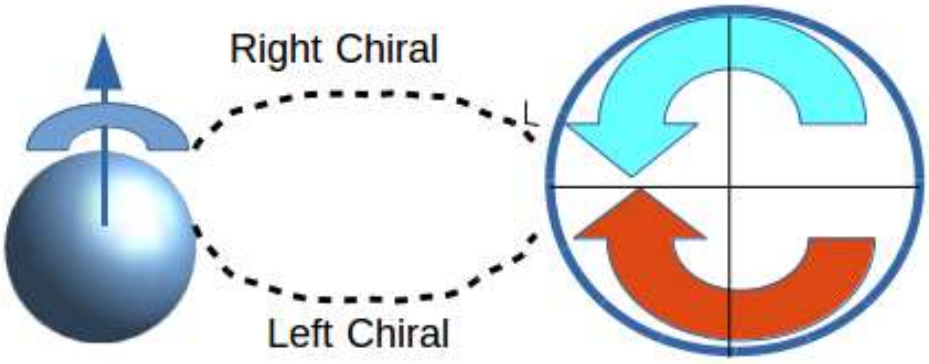

Fig. 1.4 Schematic diagram of chiral particle. Right chiral or left chiral shows the different trajectory of the particle in anticlockwise and clockwise direction respectively.

Now we further define two types of active system on the basis of whether the momentum is conserved or not.

Dry active matter:- In active matter, when a system violates the principle of momentum conservation, it is referred to as "dry" [Chaté (2020); Fily & Marchetti (2012); Marchetti et al. (2013); Shaebani et al. (2020)]. These motions include the movement of bacteria on a rigid surface, animal herds, bird flocks, and vibrating granular rods on a substrate. In all of these motions, the velocity is slowed down by the friction between the moving particles and the supporting material. In addition, the heat fluctuation reduces the hydrodynamic interactions, and the motor filament suspension and a concentrated collection of swimming bacteria may be regarded dry. The local density and orientation order parameter are the hydrodynamic fields in a dry system since both are non-zero in the broken symmetry state. The only variable that is constant in a dry system is the number of particles (ignoring death and reproduction). For example, in animal herds, cell layers, vibrated asymmetric granular particles, and films of cytoskeletal extracts are examples of dry polar systems. Vibrating granular rods and melanocyte cells on plastic surfaces are examples of dry nematic systems [Henkes et al. (2018)].

Wet active matter:- On the other hand, systems are said to as “wet” [Bär et al. (2020); Bechinger et al. (2016); Fily & Marchetti (2012); Shaebani et al. (2020)] when the active objects are suspended in a fluid, and the interaction between the particles and fluid cannot be ignored. Momentum conservation is carefully observed in a wet system. Wet nematic systems include suspensions of microtubules and motor proteins in oil, and colonies of M. Xanthus bacteria, suspensions of catalytic colloidal rods, etc. Wet polar systems include cell cytoskeleton and cytoskeletal extracts in bulk suspensions, swimming bacteria in bulk, and Pt catalytic colloids [Choudhury et al. (2017)].

1.3 Methodology

Since, the nonequilibrium systems differ from their equilibrium counterparts, there are many ways to study their distinctively complex and intriguing behavior. As there is no energy conservation in a nonequilibrium system, it is impossible to develop a suitable Hamiltonian to characterize such a system. In general, the following three approaches have been used to examine active systems in recent decades: (i) microscopic rule-based model such as the Vicsek model (VM) [Grégoire & Chaté (2004); Vicsek et al. (1995)], and also with the help of coarse-grained equations for slow variable [Bertin et al. (2006); Ihle (2011)], (ii) phenomenological technique, which comprises formulating the various terms in the equations of motion in accordance with the system's symmetry components, (iii) Lastly, the experiment that reveals the practical aspects of this system [Paxton et al. (2004)]. We will go through the specifics of these studies employed in our research in the next part.

1.3.1 Agent or microscopic rule based simulation

In the past few years, numerous uses of the potent simulation modeling technique known as microscopic rule-based modeling have been observed. In agent-based modeling (ABM), a system is represented as a group of agents, which are autonomous decision-making pseudo-particles. Based on a set of established dynamical principles, each particle updates its location and speed. To replicate the phenomenology of the active system, the dynamical rules are modified. The dynamical rules are changed to better reflect the active system's phenomenology. While finite-size particles can be guided to align with their neighbors in contact by volume exclusion or steric processes, active particles, which are symmetric in shape, move along their long body axis without any alignment interaction [Chaté et al. (2008); Fily & Marchetti (2012); Pattanayak et al. (2019); Shi & Ma (2013)]. The polar

particle interactions can be compared to the "ferromagnetic interaction" like in the spin system. Additionally, apolar particles are capable of both parallel and anti-parallel interactions. Although alignment interactions (polar/apolar) are maintained manually to simulate. But several other studies are done wherein agents are assumed to be point particles [Grégoire & Chaté (2004); Vicsek et al. (1995)]. Because the interactions between the particles are not always predictable, the SPPs tend to make mistakes while imitating their neighbors. Which is incorporated by including the noise term in the update equations [Grégoire & Chaté (2004); Vicsek et al. (1995)].

Vicsek Model (VM)

The clustering, transport, and phase change in active systems was stated with novel work of Viscek *et.al.* Vicsek et al. (1995). Vicsek model [Vicsek et al. (1995)] is based on the following criteria and is specified in two dimensions: Each SPP in the system is represented as a point-particle with direction $\theta_i(t)$ at time t and speed v_0. Later it is also studied in higher dimensions [Chaté (2020); Chaté et al. (2008)]. There is an alignment rule that operates as follows for each time step and each i^{th} particle, (i) We compute the average direction of the particles within a circle of radius r, (ii) orientation of the particle is given by the average direction of the particle θ_i plus some noise which is chosen $[-\eta, \eta]$, $\eta \in [0, \pi]$. Update equation is given by:

$$\theta_i(t+\Delta t) = arg\Big(\sum_{j \in S_i} e^{i\theta_j}\Big) + \underbrace{\delta\theta_i}_{noise} \tag{1.1}$$

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

where $r_i(t)$ is the position and $v_i(t+\Delta t)$ is the velocity of i^{th} particle as shown in Fig.1.5. Viscek model shows a order-disorder nonequilibrium phase transition for different values

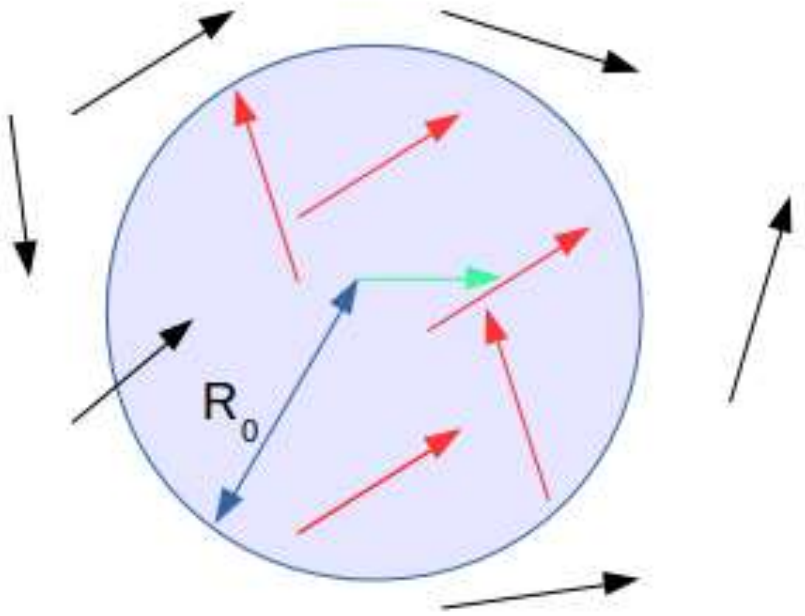

Fig. 1.5 Arrow shows different particles black particles which is outside the circle, circle which have a radius R_0 particle inside the circle shown by red arrow, final orientation of the test particle shown by green colour.

of η [Chaté et al. (2008); Grégoire & Chaté (2004); Vicsek et al. (1995)]. In this case, for higher density and small noise, the motion of the particle is ordered, which shows a continuous transition for different values of η in the presence of angular noise. In later studies it was noted that the finite-size impact is considerably more prominent, and hence the nature of the order-disorder transition becomes discontinuous when big enough system sizes are taken into account [Chaté (2020); Foffano et al. (2012)]. There are ongoing discussion on the nature of the phase transition in these systems. According to several researches, the system's update process determines the transition's character [Aldana et al. (2007)]. On

the other hand, because activity (caused by self-propulsion) indicates that the system is not in equilibrium and the Mermin-Wagner theorem does not hold, the Vicsek particles can also display a (symmetry-breaking) order-disorder transition in 2D. The Vicsek model also demonstrates several fundamental and generic characteristics of dynamical natural systems.

Langevin dynamics for active self-propelled particles

Brownian motion is the name given to the random movement of particles suspended in a media (liquid or gas), and the participating particles are known as Brownian or passive particles. Due to the surrounding medium, passive particles continuously suffer collision, and the dynamics of these collisions are stochastic in nature. The system is in equilibrium when there is a balance between dissipation and fluctuations, and this relationship is known as the fluctuation-dissipation relation (FDR) [Pathria (1996); Zemansky & Dittman (1997)]. In Newtonian dynamics, the dynamics of passive particles are narrated via stochastic and frictional terms of forces [Romanczuk et al. (2012); Van Gunsteren & Berendsen (1988)]. Langevin dynamics can therefore be used to write the Brownian particle's motion equation with Stokes frictional coefficient and a position-dependent potential U(r):

$$m\frac{d\mathbf{v}}{dt} = -\gamma\mathbf{v} - \nabla U(\mathbf{r}) + \mathbf{R}(t) \tag{1.3}$$

where **R**(t) is a delta-correlated stationary Gaussian process with mean zero, satisfying the relations $\langle R(t=0)\rangle = 0$, and $\langle R_i(t)\cdot R_j(t)\rangle = 2D_B\delta_{i,j}\delta(t-t')$, where the components $R_i(t)$ and $R_j(t)$ are referred to as Gaussian white noise with intensity D_B. Here indices i and j correspond to the Cartesian coordinates. The intensity D_B and friction coefficient γ are related by the FDR, $D_B = \gamma k_\beta T$ [Pathria (1996); Zemansky & Dittman (1997)] in the equilibrium where k_β and T represent the Boltzmann constant and temperature of the system respectively. ABPs typically have symmetrical shapes, therefore there is no

alignment interaction between them. However, the motion of these particles results in MIPS (motility-induced phase separation) [Buttinoni et al. (2013); Shaebani et al. (2020); van Damme et al. (2019)] at lower density in comparison to the passive particles. The Langevin equation is a stochastic differential equation of second order, where the first term is the damping term, the second term tells about the interaction between the particle, and the last term is the noise term in the system. We can also model the system in the overdamped regime given by the following equations:

$$\partial_t \mathbf{r}_i = v\hat{\mathbf{n}}_\mathbf{i} + \mu_1 \sum_{j \neq i} \mathbf{F}_{ij} + \sqrt{2D_t}\eta_\mathbf{i} \tag{1.4}$$

$$\partial_t \theta_i = \sqrt{2D_r}\eta_\mathbf{i} \tag{1.5}$$

s where ABPs interact with soft repulsive potential. Unit vector $\hat{n}$ determines the direction of motion of the particle. where $\hat{n} = (cos(\theta_i, sin(\theta_i))$, where θ_i is the orientation of the i^{th} particle. In eqn. 1.4 first term in the right hand side(R.H.S) comes due to activity of the particles, where v is activity of the particle. F_{ij} is short range repulsive force between the i^{th} and j^{th} particle. We can model the repulsive force in various ways like harmonic, Weeks-Chandler-Andersen(WCA), etc.[Fily & Marchetti (2012); Zeitz & Stark (2016)]. η_i represent the Gaussian white noise with mean zero and correlation is finite. Eqn. 1.5 is the orientation update equation, where nature of noise is also Gaussian with mean zero and correlation is finite.

1.3.2 Phenomenology : hydrodynamic equations of motion

The examination of symmetry-based phenomenological or hydrodynamic equations of motion is the focus of this subsection. In this section discussion involves flocking model 1.3.1 with continuum approach. Toner and Tu introduced the effective continuum theory for

the first time in 1995 [Toner & Tu (1995, 1998)]. The fundamental tenet of hydrodynamic theory contains symmetry-related concepts or conservation laws, such as those governing the conservation of mass, momentum, and energy, among others. The effective continuum model was developed by Toner and Tu based on symmetry considerations. The sole preserved field in the system is the density of active particles $\rho(r,t)$ (excluding death and birth of SPPs). The particles constantly dissipate their energy into systematic movement while moving on a frictional, dry substrate. The equation for the velocity field $\mathbf{v}$, coarse-grained density $\rho(\mathbf{r},t)$ are given by as proposed in [Toner et al. (2005)]:

$$\begin{aligned} \partial_t \mathbf{v} + \lambda_1(\mathbf{v}.\bigtriangledown)\mathbf{v} + \lambda_2(\bigtriangledown.\mathbf{v})\mathbf{v} + \lambda_3 \bigtriangledown\left(|\mathbf{v}|^2\right) = \\ \alpha\mathbf{v} - \beta|\mathbf{v}|^2\mathbf{v} - \bigtriangledown\mathbf{P} + \mathbf{D_B}\bigtriangledown(\bigtriangledown.\mathbf{v}) + \mathbf{D_T}\bigtriangledown^2\mathbf{v} + \mathbf{D_2}(\mathbf{v}.\bigtriangledown)^2\mathbf{v} + \mathbf{f}(\mathbf{r},\mathbf{t}) \end{aligned} \tag{1.6}$$

which is defined for all $\mathbf{r}$. β, D_B, D_2, and D_T are all positive, and $\alpha < 0$ in the disordered phase and $\alpha > 0$ in the ordered state. In the presence of Galilean invariance $\lambda_2 = \lambda_3 = 0$ and $\lambda_1 = 1$. $\mathbf{f}(\mathbf{r},\mathbf{t})$ term represent the noise which is Gaussian white noise correlations:

$$< \mathbf{f_i}(\mathbf{r_1},\mathbf{t_1})\mathbf{f_j}(\mathbf{r_2},\mathbf{t_2}) >= \blacksquare\delta_{\mathbf{ij}}\delta^{\mathbf{d}}(\mathbf{r_1}-\mathbf{r_2})\delta(\mathbf{t_1}-\mathbf{t_2}) \tag{1.7}$$

where Δ is constant, i, j denote Cartesian components. P is pressure which maintains the local number density from it's mean value ρ_0, $\delta_\rho = \rho - \rho_0$ given by:

$$P = P(\rho) = \sum_{n=1}^{\infty} \sigma_n(\rho - \rho_0)^n \tag{1.8}$$

Then density equation is simply the continuity equation with:

$$\frac{\partial\rho}{\partial t} + \bigtriangledown.(\mathbf{v}\rho) = 0 \tag{1.9}$$

eqn. 1.9 is conservation of bird number (not allow bird die or reproduce). Due to symmetry phenomenological coefficients λ_i, α, σ_n,β, D_i to be functions of squared magnitude $|_{\mathbf{v}}|^{\mathbf{2}}$ of the velocity, and of density ρ as well.

Up to now we model a system for active Brownian type of particles, where we have different category of the particles, like run and tumble particles, and active chiral particles. But study of a single particle moving along the bonds of a lattice is also an interesting problem to explore. Such study gives insight about the dynamics of single passive particle in different environment. System can be modelled using Lorentz lattice gas.

1.3.3 Lorentz lattice gas

Let's have a look at a class of dynamical system that simulate the motion of an object on a straightforward undirected infinite lattice L (such as an electron, an ant, a ray of light, or the Turing read/write head) which can be compared with the phenomenology of the Lorentz lattice gas (LLG) [Binder (1987); Cohen & Wang (1995); Ernst & Binder (1988); Kumar & Mishra (2019); Mishra et al. (2016); Sampat et al. (2020)]. In the models of LLG, the object moves from one site to another together with the lattice at each time step. Let some "site" of the lattice have a quenched attribute (R) that determines the object's subsequent movement on the lattice. With a set of interaction rule with the particle, R may be a mirror, rotator, or scatterer. This type of system is referred to as a Lorentz lattice gas, as shown in Fig. 1.6. LLG are straightforward microscopic rule-based models that handle a variety of physical issues, which has led to a surge in interest in recent years.

The LLG models can have mixed features rather than being solely deterministic or probabilistic. Even so, it does an excellent job of describing the dynamic progression. Even though the LLG model has a mathematical description, it is capable of solving many issues in the area of computational fluid dynamics, biochemistry, artificial life, graph theory, and

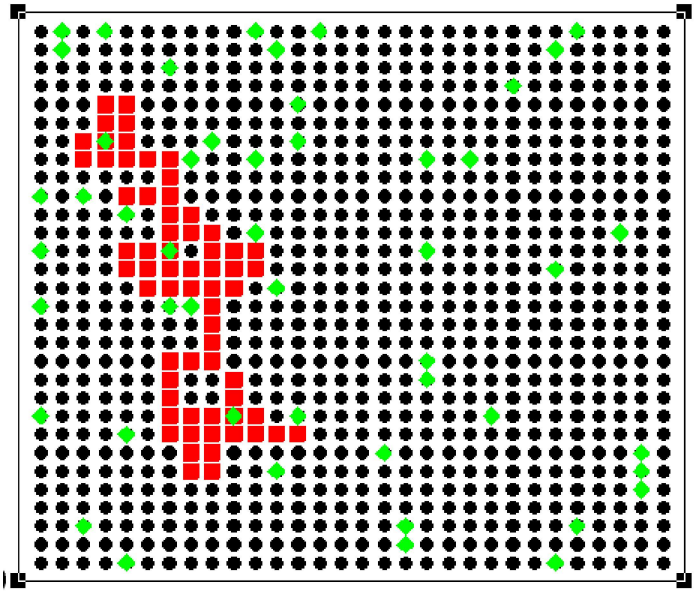

Fig. 1.6 Schematic diagram of Lorentz lattice gas. Black circle denotes the lattice point, Red rectangle denotes trajectory of the single particle, green diamond denotes the quenched rotator which rotate the motion of the particle.

theoretical computer science. Understanding the order-disorder or solid-liquid interface and researching the dynamics of aggregation, such as insect colonies, are potential uses of LLG.

The well-known Navier Stokes equation has an isotropic lattice gas variant, which was developed by Frisch *et. al.* and Wolfram. They have successfully described a simulation method for investigating complex fluids like micro emulsions in their models and derivatives. Some LLG models aid in the universal computation by simulating the dynamics of the turning machine. The goal of this thesis is to use single particle dynamics to examine the fundamental physical process known as diffusion, and the LLG models can be helpful in doing so.

A particle traveling in a Euclidean space and elastically distributed by spheres positioned randomly characterizes a classical LLG model. To comprehend the dynamics of an electron in metal and the conductivity of that metal, one uses the classical LLG model. Ehrenfest's "wind tree" model, created by P. Ehrenfest, is a simpler version. According to Ehrenfest's

model, randomly positioned diamonds with diagonals perpendicular to the coordinate axes elastically scatter traveling electrons. The two above mentioned models are considered the simplest models for examining particle diffusion in a random environment. It is challenging to analyze these models rigorously.

1.4 Objective and organisation of the thesis

Based on the system's conservation laws and symmetry components, we have covered many kinds of active matter systems in the preceding sections. We have discussed the broad framework for studying active systems and contrasted them with analogs of their equilibrium. We have discussed the bulk features of collective behavior, such as the order-disorder phase transition, long-range ordering, and phenomenology of the clean systems [Chaté et al. (2007, 2008); Marchetti et al. (2013); Ramaswamy (2010); Vicsek et al. (1995)]. We also discuss how to model a different type of particle-like active Brownian particle, the run and tumble particle, with a basic understanding of the active matter system. We have also discussed the different types of active particles where the evolution of the particle is given by the Langevin equation. In chapter 2, we study the dynamics of a collection of active particles on a two - dimensional periodic undulated surface. We observe there is a competition between the activity and surface undulation, which help us to draw a phase diagram of the system in a different regime. The Green-Kubo relation was also confirmed using two distinct methods. A detailed study is discussed in chapter 2.

Chapter 3 is dedicated to the dynamics of run and tumble particles in a binary mixture, where the evolution of the particle is given by the Langevin equation in the absence of thermal noise for active and passive particles. We observe the dynamics of the active particle always shows there is a crossover from early time ballistic to late time diffusion. Still, in the case of the passive particle, as we increase the size ratio of the particle, the

motion of the particle always goes into the subdiffusive regime. We also found crossover time for passive particles increases as we increase the size ratio of passive particles. The detailed result are discussed in chapter 3.

The chapter 4 discusses the effect of chirality on the active particles. We first characterize the dynamics of the particle for different values of chirality. We observe that as we increase the chirality of the particle motion, the particle goes into the subdiffusive regime. Based on this, we also found there are different phases in the system corresponding to different values of chirality, where the system moves from macrophase to microphase, as we further increase the value of chirality system goes into the homogeneous state. We found three different phases and the phase diagram is shown for different activity and chirality of the system. Detailed study is discussed in chapter 4.

The study of passive disk-shaped particles in the presence of active particles and calculation of the potential for different values of size ratio by using the depletion force is studied in chapter 5. As we increase the size ratio of the passive particles, the potential is much more attractive. Further, we also found that active Brownian particles in the presence of passive particles are phase separated. Detailed study discussed in chapter 5.

In chapter 6 we discuss the dynamics of a single particle moving on a random Lorentz lattice gas. The system is studied for different cases (i) particle dynamics on a random network. In this case motion of the particle shows diffusive motion. We introduce two types of rotators: (i) leftmost and rightmost and (ii) left and right. The rotators are distributed randomly in the space, In the first case, the dynamics of the particle are initially subdiffusive, and eventually, the motion goes into the superdiffusive regime. For case (ii), we found the motion of the particle shows early time diffusive to late time superdiffusive. Our study provides insight into how a single particle interacts in various environments. Detailed study discussed in chapter 6.

Finally, in chapter7, we conclude the thesis with significant remarks and future prospects

of the problems.

1.5 Technical details

The numerical results presented in the subsequent chapters have been produced by implementing numerical programmes and modeling them with the FORTRAN 77/90 compiler. The plotting tools XMGRACE and GNUPLOT have been used to produce the figures which are presented. The Institute cluster and PARAM SHIVAY computing facility at IIT(BHU) Varanasi, India, 221005 is utilized for all simulations.

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