Chapter 1

Introduction

1.1 Historical foundations of modern science

The quest to understand the nature of the universe has been a central pursuit of human thought since ancient times. Early civilizations, including those in India, made significant contributions to our understanding of the natural world. Indian scholars conceptualized the universe through the lens of Panch Tatva, or the five elements: Earth (Prithvi), Water (Jal), Fire (Agni), Air (Vayu), and Ether (Akash) [NCERT (2024); Singh (2016)]. This framework provided a holistic view of the natural world and influenced various fields, from medicine to philosophy. Aryabhata and Brahmagupta further advanced this understanding with pioneering contributions in mathematics and astronomy, developing sophisticated models of celestial movements and laying foundational principles in these fields. Their work was instrumental in shaping early scientific thought and influenced subsequent developments in various cultures [Āryabhaṭa & Clark (2018); Gupta (2008); Jha (2010)]. In the broader context, ancient philosophers such as Aristotle in Greece also proposed theories about the elements and the forces governing the cosmos, laying the groundwork for future scientific inquiry [McKeon et al. (2009); Randall & Woodbridge (1960)].

The scientific revolution of the 17th century in Europe, marked a significant turning point in our understanding of nature [Henry (1992); Redondi (1990)]. The world witnessed the advent of classical mechanics with the groundbreaking works of Isaac Newton. Newton's formulation of the laws of motion and universal gravitation provided a comprehensive framework for describing the behavior of objects and the forces acting upon them. Newtonian mechanics, or classical mechanics, described the deterministic evolution of a single particle or a system of particles under the influence of forces, revolutionizing our understanding of motion and laying the foundation for the physics that we know today [Verma (1993)]. In classical mechanics, the behavior of a single particle is governed by

Newton's laws. The state of the particle is described by its position and velocity, which evolve deterministically under the influence of forces [Mathur (2000)]. In an equilibrium state, a single particle experiences no net force, leading to a stable configuration where its macroscopic properties remain unchanged over time. As we extend our focus from a single particle to systems with many particles, the limitations of classical mechanics become evident [Aruldhas (2008); Goldstein (2011)]. In multi-particle systems, such as gases, liquids, and solids, the interactions between particles give rise to complex collective behaviors. These behaviors cannot be straightforwardly deduced from the dynamics of individual particles. For example, properties like pressure, temperature, and phase transitions emerge from the collective interactions within a system of many particles [Garg et al. (2013)]. As the 18th and 19th centuries ushered in the Industrial Revolution, the study of heat engines and the conversion of energy became increasingly important [Weinberger (2013)]. This led to the development of thermodynamics, a field that seeks to understand the principles governing energy transfers and transformations. The formulation of the first and second laws of thermodynamics, which address energy conservation and entropy, respectively, provided a macroscopic description of systems in terms of state variables like temperature, pressure, and volume [Müller (2007)].

1.2 The Emergence of Statistical Mechanics

In the late 19th and early 20th centuries, statistical mechanics emerged as a bridge between the microscopic world of classical mechanics and the macroscopic descriptions provided by thermodynamics [Grant & Phillips (2013); Uffink (2004)]. Statistical mechanics explains how macroscopic thermodynamic properties arise from the collective behavior of a large number of microscopic degrees of freedom. It introduces probabilistic concepts to describe the distribution of particles' states, leading to a deeper understanding of equilibrium and nonequilibrium phenomena [K.Huang (2008); Klein (1990); L.Boltzmann (1964); Pathria (1996); Sen (2021); Zemansky & Dittman (1997)].

Statistical mechanics aims to explain and derive macroscopic properties (such as temperature, pressure, and volume) from the underlying microscopic laws of physics (such as Newtonian mechanics for classical systems or quantum mechanics for quantum systems) [Paul M (1995)]. At the microscopic level, a system can be described by the states of individual particles (positions, velocities, spins, etc.). However, these microscopic details are too complex to be tracked individually for large systems. Statistical mechanics allows us to relate these microscopic states to macroscopic observables by considering the collective behavior of particles. For instance, instead of tracking each molecule in a gas,

statistical mechanics enables us to understand the overall temperature and pressure of the gas [Uffink (2004)].

Nonequilibrium Statistical Mechanics

In this section, we explore the intricacies of nonequilibrium statistical mechanics, highlighting the differences from equilibrium systems and introducing key concepts such as energy dissipation, detailed balance, and time-reversal symmetry.

1.2.1 Challenges in Defining Hamiltonian for Nonequilibrium Systems

In equilibrium statistical mechanics [Appendix], the Hamiltonian H provides a complete description of the system's energy, allowing for the derivation of various thermodynamic properties [K.Huang (2008); L.Boltzmann (1964); Paul M (1995); Uffink (2004)]. However, in nonequilibrium systems, the situation is more complex.

Absence of Well-Defined Hamiltonian

Nonequilibrium systems often do not have a well-defined Hamiltonian. This is because such systems are typically driven by external forces, subject to time-dependent changes, or consist of active components, which cannot be captured by a static energy function. For example:

- **Driven Systems:** Systems driven by external fields or forces (e.g., electrical currents, sheared fluids) have energy contributions that vary with time and cannot be encapsulated by a time-independent Hamiltonian [Grmela (1993)].
- **Dissipative Systems:** In systems where dissipation (e.g., friction, viscosity) plays a crucial role, the loss of energy to the environment complicates the definition of a Hamiltonian [Nicolis (1986)].
- **Active Systems:** Systems composed of active particles, such as biological cells or synthetic self-propelled particles, consume energy to perform work and exhibit behaviors that cannot be described by equilibrium statistical mechanics. These systems are inherently out of equilibrium due to continuous energy input at the microscopic level [Bechinger et al. (2016); Marchetti et al. (2013c); Ramaswamy (2010a); Toner et al. (2005a)].

1.2.2 Energy Dissipation

Energy dissipation is a hallmark of nonequilibrium systems. It refers to the process by which energy is irreversibly lost to the surroundings, typically as heat. Unlike in equilibrium systems where energy conservation is strict, nonequilibrium systems constantly exchange energy with their environment [Balakrishnan (2021)].

Dissipative Forces

Dissipative forces, such as friction or viscosity, convert organized forms of energy into thermal energy, leading to an overall increase in entropy [Skagerstam (1977)]. The presence of these forces means that energy is not conserved within the system, but rather, it is transferred to the environment.

1.2.3 Detailed Balance Condition

In equilibrium systems, the principle of detailed balance is a fundamental concept that ensures time-reversibility at the microscopic level [K.Huang (2008); Kolmogoroff (1936); Landsberg (1990)]. This principle asserts that for every microscopic process occurring in the system, there is a corresponding reverse process that occurs at the same rate. This can be mathematically expressed as:

$$W_{i\to j}P_i^{eq} = W_{j\to i}P_j^{eq}, \tag{1.1}$$

where $W_{i\to j}$ is the transition rate from state i to state j, and P_i^{eq} is the equilibrium probability of being in state i [Durrett & Durrett (1999)].

The detailed balance condition implies that the system's microscopic dynamics are such that, in equilibrium, the probability of transitioning from state i to state j is perfectly balanced by the probability of the reverse transition from j to i. As a result, there is no net flow of probability between any two states, leading to a steady state where macroscopic quantities remain constant over time [Pathria (1996)]. This is a hallmark of equilibrium systems where no currents or fluxes are present.

The physical meaning of detailed balance can be understood as a statement of equilibrium at the microscopic level: each individual process is exactly counterbalanced by its reverse, ensuring that the system does not evolve in time, as all changes are perfectly reversible. This condition is deeply tied to the second law of thermodynamics and the concept of entropy, as it implies that in equilibrium, the entropy production is zero, and the system has reached a state of maximum entropy given its constraints [Pathria (2016)].

Violation of Detailed Balance

In nonequilibrium systems, the condition of detailed balance is typically violated [Zemansky & Dittman (1997)]. This means that the transition rates between states no longer satisfy the equality expressed in Equation (1). Instead, we observe:

$$W_{i\to j}P_i \neq W_{j\to i}P_j, \tag{1.2}$$

where P_i and P_j are the nonequilibrium probabilities of states i and j, respectively [Gnesotto et al. (2018)]. The violation of detailed balance leads to net fluxes of probability between states, which manifest as non-zero currents within the system. These currents are a direct indication of nonequilibrium behavior, as they represent a continuous redistribution of probability among the system's states.

Physically, the violation of detailed balance corresponds to the system being driven by external forces or gradients, such as temperature differences, chemical potentials, or applied fields [Lebon et al. (2008)]. These driving forces break the time-reversibility of microscopic processes, leading to irreversible behavior and the production of entropy. The presence of non-zero currents is a clear signature of this irreversibility, and it is often associated with phenomena such as transport processes, chemical reactions, or the maintenance of steady states far from equilibrium.

The violation of detailed balance is central to understanding nonequilibrium statistical mechanics, where the study of such systems requires new concepts and tools, like nonequilibrium steady states (NESS), large deviation theory, and the fluctuation-dissipation theorem[Pathria (1996)].

1.2.4 Time-Reversal Symmetry

Time-reversal symmetry is a fundamental concept in equilibrium statistical mechanics, rooted in the notion that the laws of physics are generally invariant under the reversal of time [Lamb & Roberts (1998); Sachs (1987)]. If a system possesses time-reversal symmetry, its microscopic dynamics remain unchanged when the direction of time is reversed. Mathematically, this means that if we reverse the velocities of all particles and evolve the system backward in time, the system will retrace its previous states exactly, leading to a trajectory indistinguishable from the forward-time evolution [Goldstein (2011)].

This symmetry is deeply connected to the principle of detailed balance, where for every process in equilibrium, there exists a reverse process with an equal probability of occurring [K.Huang (2008)]. Consequently, in equilibrium systems, the macroscopic observables remain constant over time, reflecting the balance between forward and reverse processes.

The concept of time-reversal symmetry also plays a crucial role in the conservation laws of classical and quantum mechanics, ensuring that certain properties, such as energy and momentum, remain invariant under time reversal [Pathria (1996)].

Breaking of Time-Reversal Symmetry

In nonequilibrium systems, time-reversal symmetry is often broken, leading to irreversible processes that distinguish the past from the future [Attard (2012); De Groot & Mazur (2013)]. These systems are characterized by dynamics that do not retrace their steps when time is reversed, resulting in a clear directionality of time.

This breaking of time-reversal symmetry is most evident in processes that generate entropy and lead to the dissipation of energy. Examples include:

- **Diffusion:** When particles diffuse from a region of high concentration to a region of low concentration, the process is irreversible. If time were reversed, particles would spontaneously gather into a high-concentration region, which is highly improbable and thus indicates a break in time-reversal symmetry [K.Huang (2008)].

- **Chemical Reactions:** In a chemical reaction, reactants are converted into products, releasing or absorbing energy in the process. The reverse reaction, while possible, does not occur with the same probability as the forward reaction in non-equilibrium conditions, especially if there is an external driving force like a continuous supply of reactants. This asymmetry in the reaction dynamics breaks time-reversal symmetry [Pathria (1996)].

- **Thermal Conduction:** Heat flows spontaneously from a hotter region to a colder one, increasing the overall entropy of the system. Reversing time would imply heat flowing from cold to hot, which is forbidden by the second law of thermodynamics. This irreversible flow of heat is a clear indication of broken time-reversal symmetry [Grant & Phillips (2013)].

- **Electrical Circuits with Resistance:** In an electrical circuit with resistive components, electrical energy is dissipated as heat due to the resistance. If time were reversed, the system would require the random thermal motion of particles (i.e., heat) to spontaneously convert back into organized electrical energy, which does not happen, thus breaking time-reversal symmetry [Zemansky & Dittman (1997)].

The breaking of time-reversal symmetry in nonequilibrium systems is a key signature of their irreversible behavior. It is often associated with entropy production, where the

system evolves toward states of higher disorder. This evolution is not reversible, and it distinguishes nonequilibrium systems from their equilibrium counterparts, where time-reversal symmetry holds.

The physical implications of broken time-reversal symmetry are profound. They imply that certain processes are intrinsically directional, giving rise to the arrow of time in thermodynamic systems. This directionality is essential for understanding the behavior of systems far from equilibrium, where external forces or gradients drive the system away from its time-reversal symmetric state, leading to a steady state or dynamic behavior that is inherently irreversible [Sen (2021)].

1.2.5 Entropy Production

Entropy production is a fundamental concept in nonequilibrium systems, serving as a measure of the irreversibility of processes. Unlike in equilibrium systems, where entropy production is zero, nonequilibrium systems exhibit positive entropy production, reflecting their deviation from equilibrium conditions [Kardar (2007); Lanford (2007); Pathria (1996); Wehrl (1978)]. Entropy production can be analyzed both locally and globally. Local entropy production refers to the rate of entropy production per unit volume, providing insights into the irreversibility of processes at a microscopic level [Zemansky & Dittman (1997)]. On the other hand, global entropy production accounts for the total entropy production across the entire system, offering a macroscopic measure of the overall irreversibility of the system's dynamics [K.Huang (2008)].

1.2.6 Non-Equilibrium Steady States (NESS)

Defining NESS is crucial for understanding the behavior of systems far from equilibrium, particularly in distinguishing them from equilibrium state. In many non-equilibrium systems, despite the continuous input and dissipation of energy, the system can reach a steady state where its macroscopic properties remain constant over time. These are known as Non-Equilibrium Steady States (NESS) [Derrida (2007)]. Unlike equilibrium states, where the system has no net fluxes and is characterized by maximum entropy, NESS are maintained by a balance between the driving forces and dissipation, resulting in sustained non-equilibrium conditions [Lebon et al. (2008)].

Characteristics of NESS

- **Constant Fluxes:** One of the defining features of NESS is the presence of constant fluxes, such as the flow of energy, particles, or other conserved quantities, through

the system. These fluxes are driven by external forces or gradients, such as a temperature difference, chemical potential gradient, or external fields [Degond et al. (1998); Zamponi et al. (2005)]. For example, in a system with a constant temperature gradient, there will be a steady flow of heat from the hot region to the cold region, maintaining the system in a non-equilibrium steady state [Chattopadhyay et al. (2023)].

- **Steady-State Distribution:** Although NESS are time-independent at the macroscopic level, the underlying probability distribution of microscopic states in NESS differs from that in equilibrium. In equilibrium, the system's probability distribution is given by the Boltzmann distribution, which maximizes entropy [Pathria (2016); Stanley (1971)]. In contrast, NESS is characterized by a steady-state distribution that reflects the ongoing fluxes and the presence of driving forces. This distribution is typically not derived from a potential function and does not maximize entropy in the same way as in equilibrium [Lindblad (2001)].

In summary, while both equilibrium states and NESS represent steady state conditions, the key difference is the presence of continuous fluxes and the resulting steady-state distribution in NESS. Defining and studying NESS is essential for understanding the behavior of non-equilibrium systems, particularly in contexts where energy, matter, or other conserved quantities are continuously supplied and dissipated.

1.2.7 Fluctuation Theorems

Fluctuation theorems provide a quantitative description of the deviations from equilibrium in nonequilibrium systems. They relate the probability of entropy production in a process to the probability of entropy production in the reverse process [Ciliberto et al. (2004); Evans & Searles (2002); Evans et al. (1993); Gallavotti & Cohen (1995)].

Jarzynski Equality

One example is the Jarzynski equality [Jarzynski (1997)], which relates the free energy difference between two states to the exponential average of the work done over many realizations of a nonequilibrium process:

$$\left\langle e^{-\beta W} \right\rangle = e^{-\beta \Delta F}, \tag{1.3}$$

where W is the work done on the system, ΔF is the free energy difference, and $\langle \cdot \rangle$ denotes an ensemble average.

Crooks Fluctuation Theorem

The Crooks fluctuation theorem [Crooks (1999)] provides a relation between the probability distributions of work done in forward and reverse processes:

$$\frac{P_F(W)}{P_R(-W)} = e^{\beta(W-\Delta F)}, \tag{1.4}$$

where $P_F(W)$ and $P_R(-W)$ are the probabilities of performing work W in the forward process and $-W$ in the reverse process, respectively.

1.2.8 Examples of Nonequilibrium Systems

- **Biological Systems:** An example of a nonequilibrium biological system is the process of cellular respiration in mitochondria. Cells continuously consume glucose and oxygen to produce ATP, the energy currency of the cell, while maintaining a low-entropy state essential for cellular functions [Gnaiger et al. (1995)].
- **Transport Phenomena:** Heat conduction in a metal rod with one end heated and the other cooled is a classic example. The temperature gradient drives a continuous flow of heat from the hot end to the cold end, maintaining a nonequilibrium state as long as the temperature difference is sustained [Ván & Fülöp (2012)].
- **Chemical Reactions:** The Belousov-Zhabotinsky (BZ) reaction is a famous example of a non-equilibrium chemical reaction. It exhibits oscillating concentrations of reactants and products, with complex patterns emerging in the reaction medium due to continuous energy input and dissipation [Pechenkin & Pechenkin (2018)].
- **Active Matter:** A flock of birds is an example of active matter. Each bird (agent) consumes energy to fly, and their collective behavior results in the formation of coherent structures, such as a flock, which is sustained by the continuous input of energy from each bird's flapping wings [Marchetti et al. (2013a)].

1.3 Active Matter: A Subclass of Nonequilibrium Systems

Active matter, a fascinating subclass of nonequilibrium systems, consists of entities that consume energy to generate systematic movement or mechanical work [Bechinger et al. (2016); Bendix et al. (2008); Dombrowski et al. (2004); Marchetti et al. (2013a); Peruani et al. (2012); Rafaï et al. (2010); Ramaswamy (2010a); Szabó et al. (2006); Toner et al. (2005a)]. Examples include 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 [Dell'Arciprete et al. (2018)], animal herds [Couzin et al. (2005)], fish schools [Katz et al. (2011)], birds flocks[Ballerini et al. (2008)] , collection of cytoskeletal filaments [Ahmadi et al. (2006); Hubbard S. (2004)] such as microtubules [Sumino et al. (2012); Surrey et al. (2001)] and molecular motors, such as myosin [Joanny et al. (2007); Kron & Spudich (1986); Kruse & Jülicher (2000, 2003); Kruse et al. (2001, 2004); Kruse et al. (2005)] etc., biological systems like bacterial colonies and synthetic systems like self-propelled colloids. These systems exhibit complex collective behaviors and phase transitions that differ fundamentally from those observed in equilibrium systems.

Active matter differs from driven systems in a key aspect: the source of energy. In active matter, each particle or entity has an internal mechanism that consumes energy to produce work or motion. This intrinsic activity leads to behaviors such as swarming, flocking, and self-organization, which arise from the local interactions and energy consumption of individual components.

In contrast, driven systems are typically influenced by external forces or fields that drive the system out of equilibrium. The energy input in driven systems is applied globally, affecting all particles uniformly or through external manipulation, such as shear flows or electromagnetic fields. While both active and driven systems operate far from equilibrium, the self-propulsion and autonomous energy consumption in active matter result in unique and rich dynamical phenomena that are not present in externally driven systems.

Understanding these differences is crucial for studying the rich variety of behaviors that emerge in nonequilibrium systems, and it highlights the significance of investigating active matter to uncover novel physical principles and applications.

1.4 Types of Active particles

Active matter encompasses diverse types of particles, notably polar and nematic, each exhibiting distinct mechanisms of self-propulsion and interaction dynamics. Polar active particles, such as bacteria and motile cells, possess an inherent polarity that drives directed motion. This polarity often arises from asymmetric structures or internal processes, such as flagella-driven propulsion in bacteria or cytoskeletal dynamics in cells. The interactions among polar particles are characterized by alignment forces, where particles tend to align their orientations with their neighbors, leading to collective motion phenomena like swarming and flocking.

On the other hand, nematic active particles, exemplified by elongated rod-like structures or Janus particles with anisotropic surface properties, exhibit directional alignment without

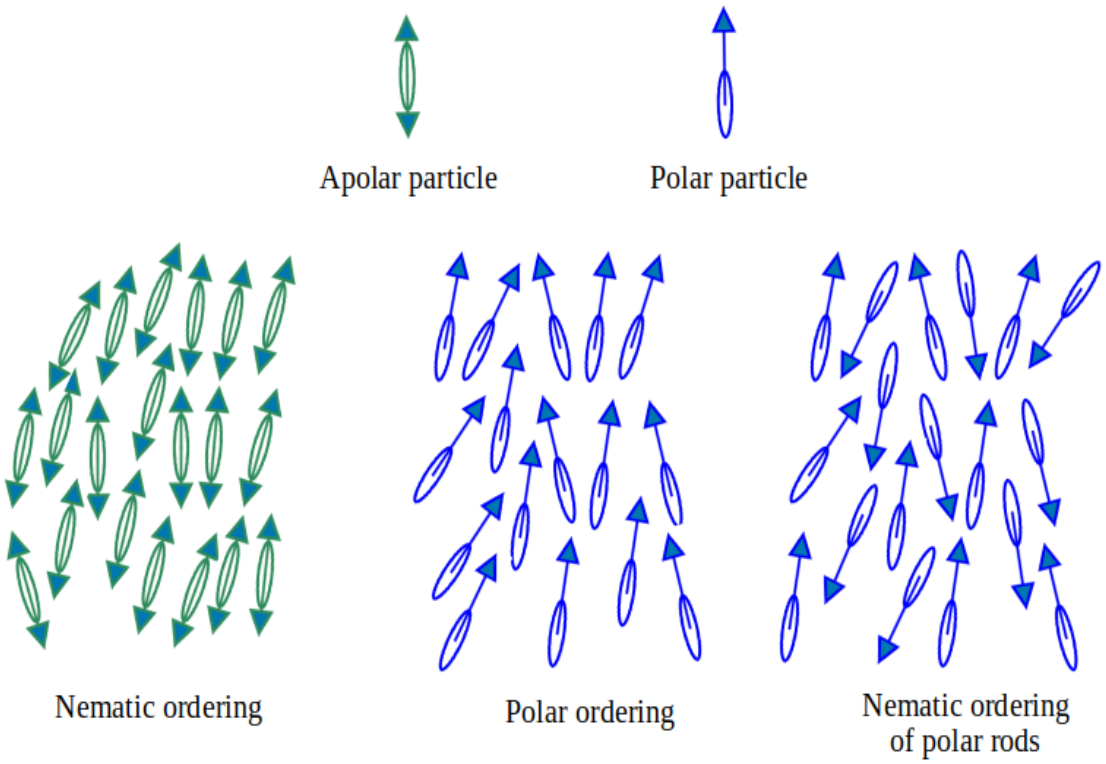


Fig. 1.1 Visualization of polar and apolar particles along with their ordering. **Apolar particle:** Apolar particle is shown with green double-headed arrows and green ellipses. The double-headed arrows indicate bidirectional alignment of the apolar particles, while the ellipses highlight their positions without directional preference. **Polar particle:** Polar particle is depicted with blue arrow and ellipse representing their head and tail respectively. The ellipses are oriented along the direction of the arrows, showing the alignment of the polar particles. **Nematic ordering:** showcasing the spatial distribution and alignment of polar particles in the system. **Polar ordering** revealing the arrangement of polar particles within the system. **Nematic ordering of polar rods:** Apolar ordering for polar particles.

a preferred direction of motion. The interactions among nematic particles are governed by long-range orientational order, resulting in complex patterns of alignment and disclination defects within the material. These particles can exhibit dynamic behaviors such as phase transitions between isotropic and nematic phases, driven by the balance between alignment forces and thermal fluctuations.

Both polar and nematic active particles interact through physical mechanisms such as steric repulsions and alignment torques, as well as through chemical signaling and environmental cues. These interactions give rise to emergent collective behaviors such as phase separation, active turbulence, and dynamic pattern formation, which are not observed in equilibrium systems or in externally driven nonequilibrium systems. Understanding the nature of these interactions is crucial for elucidating the principles governing active matter dynamics and for exploring their applications in fields ranging from materials science to biomedicine.

1.5 Models to Study Active Systems

Active systems are studied using various modeling approaches that can be broadly categorized into microscopic and coarse-grained models. These models aim to capture the dynamics and emergent behaviors of active particles at different scales of description [**?**].

1.5.1 Microscopic Models

Microscopic models provide detailed insights into the individual behaviors and interactions of active particles, accounting for their internal dynamics and interactions at a fine-grained level [Vicsek et al. (1995)].

Vicsek Model

The Vicsek model is a classic example of a microscopic model used to simulate collective motion in active matter. It describes self-propelled particles that align their velocities with nearby neighbors, leading to collective motion patterns such as flocking and swarming [Vicsek et al. (1995)].

The Vicsek model is an off-lattice model, which means it does not constrain particles to fixed lattice sites. This allows for more realistic simulations of continuous motion but at the cost of higher computational resources [Vicsek & Zafeiris (2012)].

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + v_0 \Delta t \begin{pmatrix} \cos(\theta_i(t)) \\ \sin(\theta_i(t)) \end{pmatrix}. \tag{1.5}$$

where $\mathbf{r}_i$ is the position of the i-th particle, v_0 is the constant speed, and θ_i is the orientation of i-th particle. The direction θ_i is updated as:

$$\theta_i(t+\Delta t) = \langle \theta_j(t) \rangle_{|r_j - r_i| < R} + \eta \xi_i, \tag{1.6}$$

where $\langle \theta_j(t) \rangle_{|r_j - r_i| < R}$ is the average direction of particles within a radius R, η is the noise strength, and ξ_i is a random variable with a uniform distribution [Vicsek & Zafeiris (2012)].

Langevin Dynamics

Langevin dynamics models incorporate stochastic forces to describe the Brownian motion and self-propulsion of individual particles [Romanczuk et al. (2012a)].

Similar to the Vicsek model, Langevin dynamics is also an off-lattice model, providing flexibility in particle positions and interactions. However, this also leads to higher computational demands compared to lattice-based models [Romanczuk et al. (2012a)].

The position $\mathbf{r}_i$ of the i-th particle evolves according to:

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i + \mathbf{F}_i^{\text{int}} + \mathbf{F}_i^{\text{ext}} + \mathbf{F}_i^{\text{stoch}}, \tag{1.7}$$

where $\mathbf{v}_i$ is the self-propulsion velocity, $\mathbf{F}_i^{\text{int}}$ represents interactions with other particles, $\mathbf{F}_i^{\text{ext}}$ represents external forces, and $\mathbf{F}_i^{\text{stoch}}$ is the stochastic force modeling thermal fluctuations [Romanczuk et al. (2012a)].

The stochastic force is typically modeled as:

$$\mathbf{F}_i^{\text{stoch}} = \sqrt{2D}\xi_i(t), \tag{1.8}$$

where D is the diffusion coefficient and $\xi_i(t)$ is a Gaussian white noise with zero mean and unit variance [Romanczuk et al. (2012a)].

Active Ising Model

The Active Ising model extends the classical Ising model by introducing activity-driven dynamics. Unlike the Vicsek and Langevin dynamics models, the Active Ising model is a lattice model. This means particles are constrained to fixed lattice sites, which

significantly reduces computational costs and simplifies the handling of interactions [Solon et al. (2015a)].

The movement of each spin (or particle) s_i (which can take values $+1$ or -1) to its nearest neighbor is governed by the diffusion rate $D(1+s_i\varepsilon)$, where ε is the activity parameter varying from 0 to 1. The orientation of each spin is updated using the Monte Carlo Metropolis algorithm. The Hamiltonian H for the Active Ising model is given by:

$$H = -J \sum_{\langle i,j \rangle} s_i s_j, \tag{1.9}$$

where J is the interaction strength, and $\langle i, j \rangle$ indicates summation over nearest neighbors [Solon et al. (2015a)].

Metropolis Algorithm: The Metropolis algorithm is used to update the orientation of the spins. It involves the following steps:

1. Randomly select a spin s_i from the lattice. 2. Calculate the change in energy ΔE that would result from flipping the spin s_i. 3. If $\Delta E \leq 0$, accept the flip. If $\Delta E > 0$, accept the flip with a probability $e^{-\beta \Delta E}$, where $\beta = \frac{1}{k_B T}$ (with k_B being the Boltzmann constant and T the temperature) [Solon et al. (2015a)].

By repeating these steps, the system evolves towards thermal equilibrium, while the inclusion of the activity parameter ε introduces nonequilibrium dynamics due to self-propulsion [Solon et al. (2015a)].

1.5.2 Coarse-Grained Models

Coarse-grained models simplify the description of active systems by averaging over details of individual particles, focusing instead on collective variables or mesoscopic properties [Marchetti et al. (2013c)].

Hydrodynamic Models

Hydrodynamic models treat active matter as a continuous fluid, describing the flow and interactions of density, velocity, and stress fields. These models are suitable for studying large-scale collective behaviors such as active turbulence and flow patterns in dense active suspensions [Marchetti et al. (2013a)].

The continuity equation for density $\rho(\mathbf{r}, t)$ is:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0, \tag{1.10}$$

where $\mathbf{J}$ is the total current. The total current $\mathbf{J}$ can be decomposed into two types: the diffusive current $\mathbf{J}_{\text{diffusion}}$ and the active current $\mathbf{J}_{\text{active}}$:

$$\mathbf{J} = \mathbf{J}_{\text{diffusion}} + \mathbf{J}_{\text{active}}. \tag{1.11}$$

The diffusive current $\mathbf{J}_{\text{diffusion}}$ is due to density gradients and is given by:

$$\mathbf{J}_{\text{diffusion}} = -D_\rho \nabla \rho, \tag{1.12}$$

where D_ρ is the diffusion coefficient.

The active current $\mathbf{J}_{\text{active}}$ is driven by the self-propulsion of particles and is given by:

$$\mathbf{J}_{\text{active}} = \rho \mathbf{v}, \tag{1.13}$$

where $\mathbf{v}(\mathbf{r},t)$ is the velocity field.

Navier-Stokes Equation for Velocity Field

The Navier-Stokes equation describes the dynamics of the velocity field $\mathbf{v}(\mathbf{r},t)$ in a fluid. For active matter systems, this equation can be modified to include active forces and stress. The Navier-Stokes equation is given by:

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = \frac{1}{\rho}(-\nabla P) + \nu \nabla^2 \mathbf{v} + \mathbf{f}_{\text{active}}, \tag{1.14}$$

where: $\frac{\partial \mathbf{v}}{\partial t}$ is the local acceleration of the fluid. The convection term $\mathbf{v} \cdot \nabla \mathbf{v}$ captures the transport of momentum by the fluid itself. The pressure gradient term $\frac{1}{\rho}(-\nabla P)$ ensures that the fluid responds to spatial variations in pressure, and the diffusion term $\nu \nabla^2 \mathbf{v}$ accounts for the spreading of momentum due to viscosity. $\mathbf{f}_{\text{active}}$ is the active force term, accounting for forces due to the self-propulsion of active particles

1.6 Inhomogeniety in Active sytems

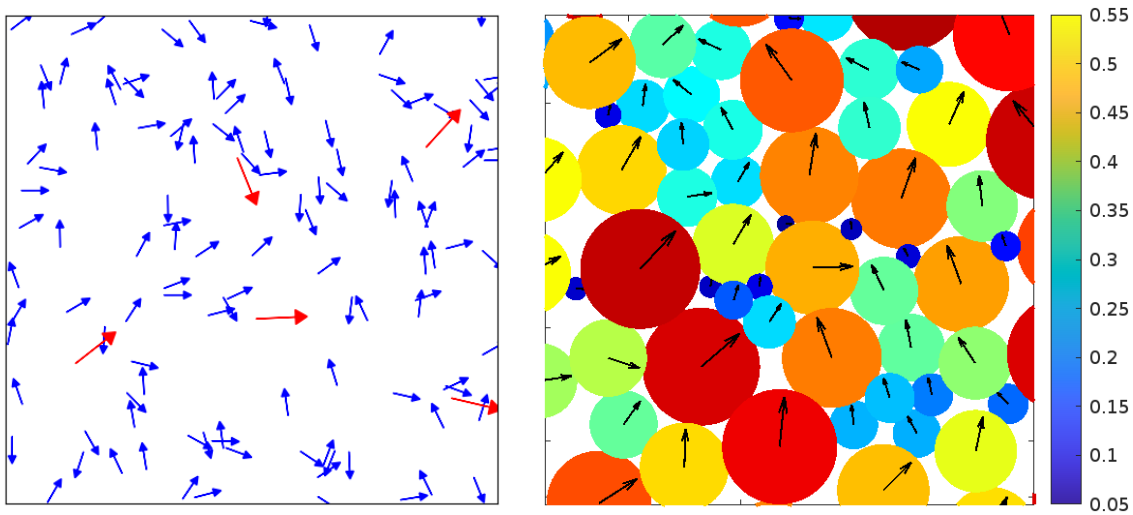
Most of the previous studies on dynamic and steady state properties of active matter systems, focuses on systems in clean or homogeneous medium [Mishra & Mishra (2023); Pattanayak & Mishra (2018a); Toner & Tu (1995, 1998a); Toner et al. (2005b)]. But disorder or inhomogeneity are inevitable in nature [Chepizhko & Peruani (2013); Mishra et al. (2023); Morin et al. (2017b); Reichhardt & Reichhardt (2017); Yllanes et al. (2017)]. Some of the recent studies have shown the effect of disorder on the ordered state of polar

self-propelled particles in two and three dimensions [Chepizhko & Peruani (2013); Das et al. (2018a); Morin et al. (2017b); Quint & Gopinathan (2015); Sándor et al. (2017b); Singh et al. (2021a,b); Yllanes et al. (2017)]. It is observed that disorder can break the robust long ranged ordered state in two-dimensions and changes it to quasi-long ranged order. Whereas in three-dimensions, the ordering remains unaffected by the presence of disorder.

Inhomogeneities within a system can be classified into two types: intrinsic and extrinsic. Intrinsic inhomogeneities arise from the inherent variations between individuals, such as differences in their structure, activity levels, and responses to their environment. On the other hand, extrinsic inhomogeneities stem from the external environment, including factors like spatial gradients in temperature or chemical concentrations, as well as physical obstacles. This section explores the impact of both types of disorder on active systems, with a particular emphasis on how these inhomogeneities influence the dynamics of individual particles and their collective behavior, including pattern formation, ordering kinetics, and phase transitions. Recent studies highlight the critical role that inhomogeneities play in shaping the behavior of active systems under random perturbations. By engineering disorder in active systems, it is possible to control their behavior for various applications, such as drug delivery, microrobotic devices, and granular industries.

1.6.1 Extrinsic Inhomogeneity

Extrinsic disorder is introduced into the system from the environment. For example, in Vicsek-like models, obstacles in the medium can be modeled as random quenched rotators, representing extrinsic disorder Das et al. (2018a, 2020). A schematic of a system containing point-like self-propelled particles (SPPs) on a two-dimensional substrate, along with disorder or random quenched rotators with random and fixed orientations, is illustrated in Fig. 1.2(a). Physical obstacles in the path of the particles can also constitute extrinsic disorder, directly affecting the orientation of incoming particles. In this context, disorders function like random "road signs" that dictate the direction of motion of the SPPs. Additionally, the disorder can be either completely quenched in time or influenced by the flow of particles, leading to changes in its properties. For instance, a moving crowd might alter the orientation of a random rotator or slightly displace it. In the first scenario, where the disorder is randomly placed but does not change over time, it is referred to as quenched disorder. In the second scenario, where particles can affect the disorder, it is called non-quenched disorder. Quenched disorder can be introduced as an additional random orientation in space that does not evolve with time in Eq. 1.6, while non-quenched disorder can be modeled as a random disorder term in Eq. 1.6 with an additional equation



(a) Extrinsic inhomogeneity. (b) Intrinsic inhomogeneity.

Fig. 1.2 A cartoon of a particular type of Extrinsic and Intrinsic inhomogeniety in panel (a) and (b) respectively. The red arrows (in (a)) are the random quenched directions and blue arrows (in (a)) are orientation of particles. The colors of the circle in (b) represents their size and arrows on the circle are the orientation of particles.

governing its time evolution. In the hydrodynamic equations, Eq. 1.10 and Eq. 1.14, this is equivalent to introducing a random force that is either fixed in time or has a memory with respect to time. The effects of both random quenched and non-quenched disorder will be discussed in the results section. The following section will describe intrinsic disorder.

1.6.2 Intrinsic Inhomogeneity

Intrinsic disorder originates from the inherent properties of the particles themselves. For instance, particles may differ in size Kumar & Mishra (2022), self-propulsion speed Pattanayak et al. (2020), experience different levels of thermal fluctuations, or interact with varying strengths Singh et al. (2021b). Figure 1.2(b) illustrates a system of active Brownian particles (ABPs) with varying radii, where the color of each circle represents the particle's radius, and the arrows indicate their direction of motion.

Intrinsic disorder is typically characteristic of the particles and is generally unaffected by the surrounding environment. This is understandable, as not all particles within a given system are necessarily identical in their properties; natural variations can occur. If the properties of particles were to evolve due to environmental influences, they would no longer be considered disordered.

Recent experiments have shown that the speeds of *B. Subtilis* bacteria within a collective are not constant but rather distributed over a broad range. This finding suggests that the constant speed assumption used in the Vicsek model requires modification. Additionally, recent studies have demonstrated a log-normal speed distribution among bacteria in a collective. Inspired by these observations, one can introduce a speed distribution for particles in the simple Vicsek model (*SVM*). In a minimal approach, particle speeds can be drawn from a Gaussian distribution with a finite mean and variance. The variance of this distribution is a crucial parameter of the model; when the variance is zero, the model reduces to the standard *SVM*.

1.7 Observables to characterize the system:

1.7.1 Ordering in the System

In active systems, the concept of ordering plays a significant role in understanding their collective behaviors. Ordering can manifest in various forms, from short-range correlations to long-range order (LRO). In the context of active matter, particularly dry polar active fluids, the behavior of order and its stability can differ markedly from that observed in equilibrium systems [Cugliandolo & Gonnella (2018)].

Long-Range Order (LRO)

Long-range order (LRO) in a system refers to the state where the velocities $\vec{v}_i$ of individual particles are aligned over large distances, leading to a non-zero average velocity, $\langle \vec{v}_i \rangle \neq 0$. This implies that the particles, on average, point in the same direction, forming a coherent, ordered state [Das et al. (2018a); Toner et al. (2018a)].

Mermin-Wagner Theorem

The Mermin-Wagner theorem states that continuous symmetries cannot be spontaneously broken at finite temperature in systems with dimensions $d \leq 2$. This implies that in two-dimensional equilibrium systems with continuous symmetries, long-range order cannot exist at finite temperatures due to the presence of thermal fluctuations that destabilize the ordered state [Halperin (2019)].

Applicability to Active Systems

The Mermin-Wagner theorem, however, does not apply to active systems, specifically dry polar active fluids. These systems can develop long-range order even in two dimensions. This deviation arises because active systems are inherently out of equilibrium due to the continuous input of energy at the microscopic level, which drives persistent motion and

can stabilize ordered states against fluctuations that would otherwise destroy them in equilibrium conditions [[Solon et al. (2015a); Toner et al. (2005b)].

1.7.2 Ordering in Different Dimensions

The behavior of ordering in equilibrium and active systems, with and without disorder, varies across different dimensions is shown in Table.1.1. In equilibrium systems, the nature of the ordering is largely influenced by thermal fluctuations, with Long-Range Order (LRO) being possible in three dimensions [Toner et al. (2018a)], but only Quasi Long-Range Order (QLRO) or Short-Range Order (SRO) in two and one dimensions, respectively [Das et al. (2018a); Mishra et al. (2024)]. In contrast, active systems, particularly those that are clean and free of disorder, demonstrate a remarkable ability to achieve LRO even in lower dimensions, such as 2D and 1D. This is a key distinction between active and equilibrium systems, highlighting the unique dynamics of active matter where continuous energy input at the microscopic level supports sustained ordering. However, the introduction of disorder in active systems can disrupt this ordering, leading to QLRO in 2D and leaving the behavior in 1D still an area requiring further exploration.

Dimension	**Equilibrium system T $\neq$ 0**	**Active system (clean)**	**Active systems with disorder**
3D	LRO	LRO	LRO
2D	QLRO	LRO	QLRO
1D	SRO	LRO	Not studied

Table 1.1 The table presented provides a detailed comparison of ordering phenomena in equilibrium systems $T \neq 0$, clean active systems, and active systems with disorder across different spatial dimensions. The ordering behavior is categorized into Long-Range Order (LRO), Quasi Long-Range Order (QLRO), and Short-Range Order (SRO).

1.7.3 Phase Transition

Phase transitions are fundamental phenomena in both equilibrium and nonequilibrium systems, marking changes in the state of matter or the order of a system as external conditions such as temperature, pressure, or interaction strength are varied [Pathria (2016); Paul M (1995)].

Equilibrium Phase Transitions

In equilibrium systems, phase transitions are well-studied and occur in various forms, each characterized by a distinct change in the state of matter or order within the system. A classical example is the transition from solid to liquid to gas, where matter changes state with increasing temperature or decreasing pressure. Another well-known transition is the ferromagnetic to paramagnetic transition, which occurs in magnetic materials as the temperature is raised above the Curie point, causing the system to lose its spontaneous magnetization and become paramagnetic. Similarly, in superconducting materials, a superconducting phase transition occurs, where the material enters a state with zero electrical resistance below a critical temperature. Liquid crystals exhibit multiple phase transitions, such as the change from an isotropic to a nematic to a smectic phase, with increasing order as the temperature is lowered. Lastly, the ferroelectric to paraelectric transition involves a shift from a ferroelectric phase, characterized by spontaneous electric polarization, to a paraelectric phase, where the material loses its spontaneous polarization at higher temperatures [Pathria (2016)].

Types of Phase Transitions

Phase transitions can be categorized into two primary types based on their characteristics:

- **First Order / Discontinuous Phase Transition:** In these transitions, there is a coexistence of the two phases at the threshold. Examples include the solid-liquid transition where both solid and liquid phases coexist at the melting point. These transitions are typically characterized by a latent heat and discontinuous changes in the order parameter.
- **Second Order / Continuous Phase Transition:** These transitions are marked by a continuous change in the order parameter, with the two phases on either side of the transition becoming indistinguishable as the threshold is approached. Critical phenomena such as scaling laws and diverging susceptibilities are often observed near these transitions. An example is the ferromagnetic to paramagnetic transition where the magnetization continuously decreases to zero at the Curie point.

Phase Transitions in Active Systems

Active systems, which are inherently out of equilibrium, can also exhibit phase transitions, but their nature and classification can differ significantly from those in equilibrium systems. The continuous input of energy and persistent motion in active matter can lead to novel

behaviors and transitions that do not conform to the classical equilibrium classifications. Understanding these transitions requires a framework that accounts for the unique driving forces and interactions present in active matter [Bhattacherjee et al. (2015); Chaté et al. (2008); Mishra & Mishra (2022)].

1.8 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 2, a minimal lattice model of self-propelled polar particles with birth and death on a two-dimensional substrate is introduced. The system shows a disorder-to-order transition, influenced by temperature and birth-death parameters, transitioning from first-order to continuous types.

3 explores quenched disorder effects on self-propelled particles in one dimension, showing how disorder density impacts macroscopic ordering and clustering, leading to particle localization around disorder.

4 examines Active Brownian Particles (ABPs) on substrates with space-dependent activity. The system's dynamics and steady state are studied for various activity profiles, revealing particle density profiles that mimic substrate inhomogeneities.

In 5, a model coupling polar and apolar species (liquid crystals) is presented. The coupling leads to string formation connecting defects, visible in the order parameter fields of both species, acting as domain walls separating oppositely oriented domains. Defect pairs connected by strings can be same or opposite in nature.

1.9 Technical details

The numerical results discussed in the upcoming chapters are obtained by writing the numerical codes and simulated using the FORTRAN 90/95 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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