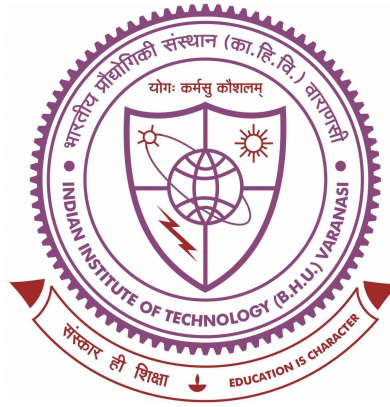


# EXTENDED ABSTRACT

## Dynamics and phases of active nematics, active Brownian particles with inhomogeneity and particle in Lorentz lattice gas



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## Abstract

Living organisms like birds flock, fish school, bacteria, cytoskeletal filaments inside an animal cell, etc., share various complex features. They show collective motion and collision, unusual structural pattern formation, robust mechanical properties, etc. One of the characteristic properties of these organisms is that each object take the energy from its surroundings and use it for motion. We generally call these objects “active objects,” and such systems are called “active matter”. Almost every living organism can be called “active matter”, making it an important research area to explore. The study of active matter can unearth many exciting and essential properties that can help design similar systems in the lab. The knowledge of active matter can be extended to solve many biological complexities like targeted drug delivery inside the human body, understanding the complex and vital phenomenologies of living organisms, different rheological properties of cells in a tissue, etc. There has been significant progress in understanding different physical phenomena like collective behavior in various active systems. The active systems have many exciting properties, e.g., long-range order, giant density fluctuation, etc. When quenched from a disordered state where active objects (or particles) are randomly oriented to an ordered state, the ordering occurs via some *specified interaction rule* among active objects, leading to the ordered domain’s formation. These ordered domains grow with time, and the system achieves a state where all the particles orient themselves in one direction. For example, a flock of birds travel thousands of miles without deviating from their path, which is possible only because of the long-range ordering in the flock. Further, the ordered state in an active system can be affected by the presence of intrinsic/extrinsic inhomogeneity. Inhomogeneity in an active system can appear in two ways: one, obstacles in the path of active particles, called extrinsic inhomogeneity; second, intrinsic inhomogeneity when the active objects can differ in their size, self-propulsion speed etc. The study of active matter has been an emerging field of research in recent years that

requires a vast understanding of statistical physics. Estimating the exact amount of energy taken for motion and collision in an active system is nearly impossible. Due to a non-zero flow of particles current in active matter, system never reaches a *true* equilibrium. Hence, these systems do not follow the usual formalism of equilibrium statistical mechanics, known as the nonequilibrium systems. Understanding the broad range of nonequilibrium phenomena in terms of their statistical and thermodynamic framework of active matter is an emerging area of current research.

Many other systems show complex features like diffusion of a particle in a complex environment, transport of particles through a narrow channel, growth of forest, etc. such problems can be studied without worrying about the particle-to-particle interactions among the individual objects. Also, these problems can be solved using the standard tools of equilibrium statistical mechanics. Hence, the Lorentz lattice gas model, where particles move along the bonds of a lattice, is one way to study such a system with noninteracting particles.

This thesis addresses many fundamental problems related to active matter with inhomogeneity, where the particles have some specified interaction. Further, we study the behavior of noninteracting particles in a complex environment using the Lorentz lattice gas model. We divide this thesis into two parts; the first part covers active matter, where particles are self motile and interact via some fixed interaction rule. In the second part, we address the problem of the Lorentz lattice gas, where particles are noninteracting. We organize the thesis according to the following chapters:

**Chapter 1** is dedicated to the introduction to the active matter system and the Lorentz lattice gas. We give a detailed introduction about the existing literature, motivation, and importance of the work presented in this thesis. This chapter provides a thorough understanding of the active matter system and methods to study them. Further, we offer a detailed description of the Lorentz lattice gas model and the motion of noninteracting particles in it.

In **Chapter 2**, we introduce a *two* dimensional active nematics with quenched disorder. We write the coarse-grained hydrodynamic equations of motion for slow variables, *viz.* density and orientation. Disorder strength is tuned from zero to large values. Results from the numerical solution of equations of motion as well as the calculation of two-point orientation correlation function using linear approximation show that the ordered steady state follows a disorder-dependent crossover from quasi long-range order (QLRO) to short-range order (SRO). Such crossover is due to the pinning of  $\pm 1/2$  topological defects in the presence of finite disorder, which breaks the system in uncorrelated domains. Finite disorder slows the dynamics of  $+1/2$  defect, and it leads to slower growth dynamics. The two-point correlation functions for the density and orientation fields show good dynamic scaling but no static scaling for the different disorder strengths. Our findings can motivate experimentalists to verify the results and find applications in living and artificial apolar systems in the presence of a quenched disorder.

In **Chapter 3**, we introduce *two* dimensional active nematics suspended in an incompressible fluid, with quenched disorder. We write the coarse-grained hydrodynamic equations of motion for slow variables, *viz.* density field, flow field, and orientation field. The disorder is introduced in the orientation field, which interacts with the local orientation at every point with some strength. Disorder strength is tuned from zero to large values. We numerically study the system's kinetics and find that the finite disorder slows the ordering kinetics. For all disorders, the system shows the dynamic scaling, whereas no static scaling is found for different disorders. Disorder slows the kinetics of the growing domains, but the effect of disorder on the density growth is relatively smaller than that of the orientation field. The effect of disorder is almost the same for both contractile and extensile cases.

In **Chapter 4**, we numerically study the dynamics and the phases of self-propelled disk-shaped particles of different sizes with soft repulsive potential in two dimensions. Size

diversity is introduced by the polydispersity index (PDI)  $\varepsilon$ , which is the width of the uniform distribution of the particle's radius. The self-propulsion speed of the particles controls the activity  $v$ . We observe enhanced dynamics for large size diversity among the particles. We calculate the effective diffusion coefficient  $D_{eff}$  in the steady-state. The system exhibits four distinct phases, jammed phase with small  $D_{eff}$  for small activity and liquid phase with enhanced  $D_{eff}$  for large activity. The number fluctuation is larger and smaller than the equilibrium limit in the liquid and jammed phase, respectively. Further, the jammed phase is of two types: solid-jammed and liquid jammed for small and large PDI. Whereas the liquid phase is called motility induced phase separation (MIPS)-liquid for small PDI and for large PDI, we find enhanced diffusivity and call it the *pure liquid* phase. The system is studied for three packing densities  $\phi$ , and the response of the system for polydispersity is the same for all  $\phi$ 's. Our study can help understand the behavior of cells of various sizes in a tissue, artificial self-driven granular particles, or living organisms of different sizes in a dense environment.

In **chapter 5**, we study the dynamics of a particle moving on one-dimensional Lorentz lattice-gas where particle performs mainly three different kinds of motion *viz* ballistic motion, normal diffusion, and confinement. There are two different types of scatterers, *viz* reflector and transmitters, randomly placed on the lattice. Reflectors are such that they reverse the particle's velocity direction, and the transmitters let it pass through. Scatterers also change their character with flipping probability  $1 - \alpha$  once particles pass through. Hence the system is defined by two sets of parameters  $r$ , which is the initial density of reflector/transmitter and  $\alpha$ , the probability of flipping. For  $\alpha = 0$  and  $\alpha = 1$ , dynamics of the particle are purely deterministic; else, it is probabilistic. In the pure deterministic case, the dynamics of the particle is either propagation in one direction or confined between two nearby reflectors present. For the probabilistic case  $\alpha \neq 1$  and  $\neq 0$ , although the dynamics of particles show anomalous diffusion where dynamics is faster, slower, and comparable to normal diffusion on the variation of system parameters

$(\alpha, r)$ , but the asymptotic behavior of the particle is normal diffusion. We plot the phase diagram for the asymptotic behavior in the plane of  $\alpha$  and  $r$  and estimate phase boundaries.

In **chapter 6**, we study the dynamics of a particle moving in a square two-dimensional Lorentz lattice-gas. The underlying lattice-gas is occupied by two kinds of rotators, “right-rotator (R)” and “left-rotator (L)” and some of the sites are empty viz. vacancy “V”. The density of  $R$  and  $L$  are the same and density of  $V$  is one of the key parameters of our model. The rotators deterministically rotate the direction of a particle’s velocity to the right or left and vacancies leave it unchanged. We characterise the dynamics of particle motion for different densities of vacancies. Since the system is deterministic, the particle forms a closed trajectory asymptotically. The probability of the particle being in a closed or open trajectory at time  $t$  is a function of the density of vacancies. The motion of the particle is uniform throughout in a fully occupied lattice. However, it is divided in two distinct phases in partially vacant lattices: The first phase of the motion, which is the focus of this study, is characterised by anomalous diffusion and a power-law decay of the probability of being in an open trajectory. The second phase of the motion is characterised by subdiffusive motion and an exponential decay of the probability of being in an open trajectory. For lattices with a non-zero density of vacancies, the first phase of motion lasts for a longer period of time as the density of vacancies increases.

**Chapter 7** contains a summary of the entire scientific work of this thesis. And, we discuss the future prospects of the problems and their extensions to have further practical application.