Chapter 5

Collection of self-propelled particles across an order-disorder interface

5.1 Introduction

In the previous chapter.4, we have studied the effect of bond disorder near to the order-disorder transition. We observe continuous phase transition and system information entropy increases with increasing inhomogeneity. Hence inhomogeneity promotes faster information transfer in the system. The collective behavior of self-propelled particles is an active area of the current research. Their collective range varies from a small intercellular scale [Kron & Spudich (1986); Laub & Loomis (1998); Ndlec et al. (1997); Takiguchi (1991)] to a much larger scale [Bonner (1998); Chen et al. (2019); Giblin (1999)]. In 1995, T. Vicsek introduced a minimal model for these systems [Vicsek et al. (1995)]. In the same year, Toner and Tu [Toner & Tu (1995)] explained collective behaviour of self-propelled particles or polar flock by using the hydrodynamic equations of motion by considering the symmetry elements of the system. In the Vicsek study, each individual is modeled as a point particle moving along their heading direction with a constant speed and align through a short-range alignment interaction with their neighbors on a two-dimensional substrate. The results show long-range ordering and order-disorder transition in these systems; however, it depends on the system parameters like density and randomness present in the system.

In the last few years, scientists have shown their interest in studying the behavior of active particles at the interface of two different substrate mediums [Dietrich et al. (2017)]. In most of these studies, active Brownian particles are considered, and two different substrate mediums are different liquids. Basically, these types of systems are modeled to mimic the colloidal suspensions [Buttinoni et al. (2013); Palacci et al. (2013); Theurkauff et al. (2012)] and their characteristic behavior. In a recent study, Dietrich et al. [Dietrich et al. (2017)] have considered the two-dimensional nature of the active Brownian motion of catalytic microswimmers at solid and liquid interfaces and they found that particles that are trapped at the fluid-fluid interface swim with high or low velocities depending on the Pt cap orientation at the interface and their reorientation time depends on the medium. Further, 2D-confinement at fluid-fluid interface gives rise to a unique distribution of swimming velocities: the patchy colloids uptake two main orientations leading to two-particle populations with velocities that differ by order of magnitude [Dietrich et al. (2017)].

Besides these interesting studies, scientists have not paid much attention to study, how does a polar flock react at the interface of the two medium, which is very much analog to the Josephson junction, an equilibrium analogous. Where junction is made of insulating and two sides are conducting material. Further, the conducting material can be thought of as an ordered flock of electrons where electrons move coherently, while the insulating region behaves as a disorder flock of electrons.

In the same fashion, we have modeled a system of polar self-propelled particles (SPPs) with Vicsek type interaction through a thin rectangular narrow channel in the two-dimensional substrate with periodic boundary conditions. Further, the thin channel is divided into three

sides wherein the region of leftmost and rightmost sides SPPs are in the deep ordered state, and in the middle region SPPs are in high disordered state. The intermediate disorder region is also called as junction. The system is studied in rectangular channel. In some studies for comparison, a small external field (which encourage particles to align in the direction of field) is applied along the long axis of the channel. This system is referred to as a system with perturbation. Most of the studies are performed without, any external field and system is referred to as without perturbation. System is studied for different widths of the intermediate disorder region. On tuning the width of the disorder region, flock with perturbation shows a strong dependence on the width of the region whereas system without perturbation shows small change with respect to the width of the disorder region. At the junction, we have found the current reversal [Kontos et al. (2002)] for a critical width of the junction, which is a common feature of the Josephson junction. Further, the particle current at the junction decreases with an increase in the junction width.
The rest of the chapter is organized as follows. In the section 5.2 we discuss details about the model. Further, in section 5.3 we discuss the results, and finally, in section 5.4 we conclude the chapter with a summary and discussion.

5.2 Model

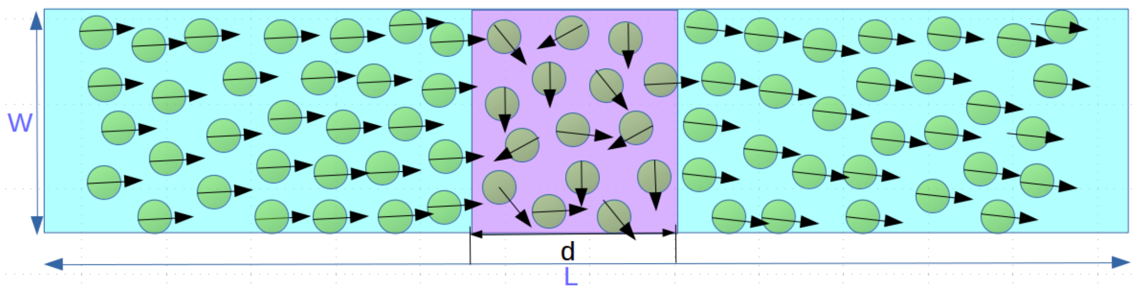

Fig. 5.1 (color online) We show a cartoon picture of the model. Left and right most box show the particles (SPPs) with arrows are, in the deep ordered state. Middle section shows the particles in disordered state. Noise strength for middle region $\eta = 0.7$ and for rest of the region $\eta = 0.3$

We consider a collection of polar self-propelled particles moving on a two-dimensional substrate on a rectangular narrow channel with periodic boundary condition (PBC). The width and long axis of the channel are defined by W and L, respectively. Particles interact through a short-range alignment interaction within a small interaction radius R_0. Moreover, the strength of interaction of each SPP is the same. The system is divided into three regions viz; two sections on the left and right sections represent the ordered region of the SPPs and third middle section shows the disordered region of the SPPs respectively. The cartoon of the model is shown in Fig.5.1. The width of the junction is varied $d = 1, 2, 3....$ and 20. In three regions, each particle is defined by its position $\mathbf{r}_i$ and orientation θ_i, and they move along the direction of their orientation with a fixed speed $v_0 = 0.5$. All the particles are updated by the position $\mathbf{r}_i(t)$ and the orientation $\theta_i(t)$ at time t are given as,

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + v_0 \mathbf{n}_i \Delta t \tag{5.1}$$

$$\mathbf{n}_i(t+\Delta t) = \frac{\sum_{j \in R_0} \mathbf{n_j}(t) + \eta_k N_i(t) \xi_i(t)}{w_i(t)} \tag{5.2}$$

Where, $\Delta t = 1.0$ is the small-time step and $\mathbf{n}_i = (\cos\theta_i, \sin\theta_i)$ is the unit direction vector of the i^{th} particle on the two-dimensional rectangular substrate. In Eq $\sim$5.2, the first term in the R.H.S represents the short-range alignment interaction inside the interaction radius (R_0) of the i^{th} particle. The second term $\xi_i(t)$ in the R.H.S of Eq $\sim$5.2 denotes the vector noise (unit random vector), which measures the error made by a particle, following its neighbors. $N_i(t)$ denote the number of neighbors within the interaction radius of the i^{th} particle at time t. Further, η_k (k=1,2) shows the strength of the randomness present in the system. η_1(0.3) and η_2(0.7) are the strength of random noises in ordered and disordered regions respectively. The above values of noise is chosen, because in the clean polar flock in bulk with vector noise, the order-disorder transition happens at $\eta \sim 0.6$ (for the fixed parameter used here) [Chaté et al. (2008); Singh et al. (2021)]. $w_i(t)$ is the normalisation factor which reduces the R. H. S. of the Eq $\sim$5.2 to a unit vector. Some of the results are also are obtained by adding an external field along the long axis of the channel; hence the orientation update equation will become $\mathbf{n}_i(t+\Delta t) = \frac{\sum_{j\in R_0}\mathbf{n_j}(t)+h_0\mathbf{n_p}+\eta_k N_i(t)\xi_i(t)}{w_i(t)}$, the strength of the external field is kept fixed to a small value h_0 with direction $\mathbf{n_p} = (1,0)$. After the above equation: this model systems is referred to as system with perturbation, whereas without such an external field system is referred as without perturbation. Further, system density is defined by $\rho = \frac{N}{L\times W} = 1.0$ where N is the total number of particles in the system. All the particles are allowed to move throughout the system, either it is order or in disorder regions but in both regions, they experience the noise of different regions. All the results discussed below are in the steady state, and total time step of the simulation is taken by 10^6. One simulation step is counted after the update of all the particles once.

5.3 Results

5.3.1 Steady state behaviour

Effect of junction on global orientation order parameter

First, we study the effect of junction width d on the global orientation in the whole system of size $L\times W = 200\times 5$ for different junction width d. Ordering in the system is characterized by the mean orientation order parameter,

$$\Psi(t) = \frac{1}{N}|\sum_{i}^{N} n_i(t)| \tag{5.3}$$

In the ordered state, i.e., when majority of particles are moving in the same direction, then Ψ will be closer to 1, and of the order of $\frac{1}{\sqrt{N}}$ for a random disordered state. First, we show the variation of Ψ for system without perturbation. In fig.5.2(a), we plot Ψ vs. width of

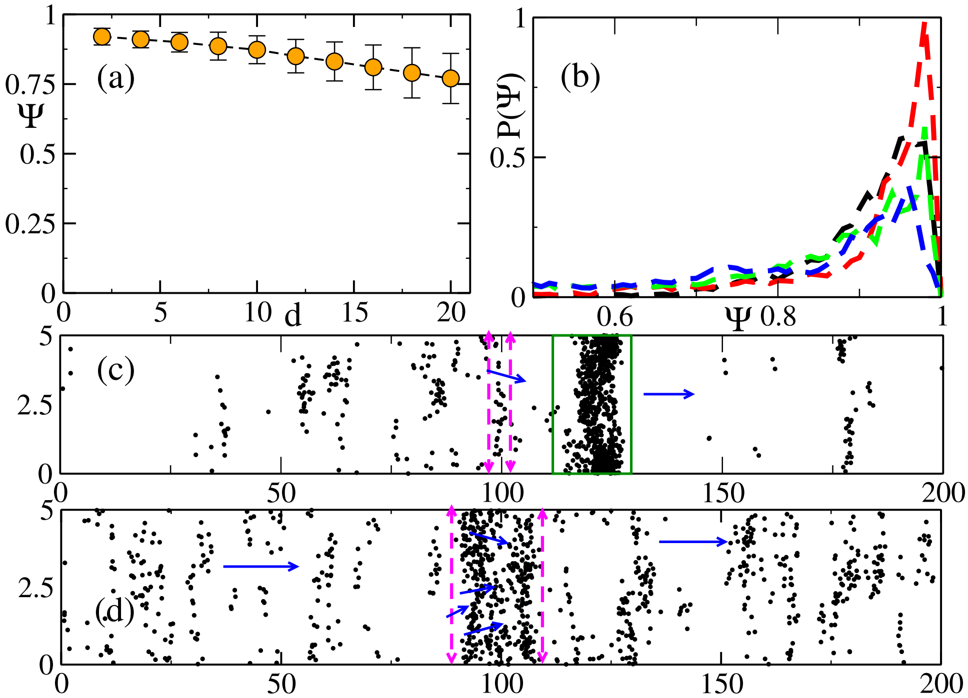

Fig. 5.2 (color online) All the plots (a)-(d) shown here for without perturbation. (a) We plot the global orientation order parameter Ψ vs. width of the disorder region d. (b) Plot shows the global order parameter distribution $P(\Psi)$ for different width of the junction 'd'. Different colored break lines are for d=4 (black), d=8 (red), d=12 (green) and d=18 (green). Plot (c) and (d) show the space snapshots of the system for width d=2 and 18 respectively. Pink line shows the boundry of the junction and blue lines with arrow show the mean orientation of the local flock. $L \times W = 200 \times 5$ and $\rho = 1.0$

the junction 'd' and found that with increase d, Ψ shows small decays, which have been further confirmed by orientation distribution $P(\Psi)$ in fig5.2(b). To confirm the small decay of Ψ, we have shown the snapshots for different junction widths 'd=2 and 16' in fig.5.2(c) and (d), respectively. For lower width junction 'd=2', SPPs form a coherent band and pass the junction without disturbing their orientation fig5.2(c). Furthermore, for the higher width of the junction, within the junction particles are aligned in the same direction, leads the higher values of Ψ in fig.5.2(d). But a small change in the Ψ with the increase in 'd', is because particles inside the junction are less coherent.

Further, we have studied the system with external perturbation in the flock. The perturbation introduced in such a way that flock is biased to move along the long axis. Interestingly, we

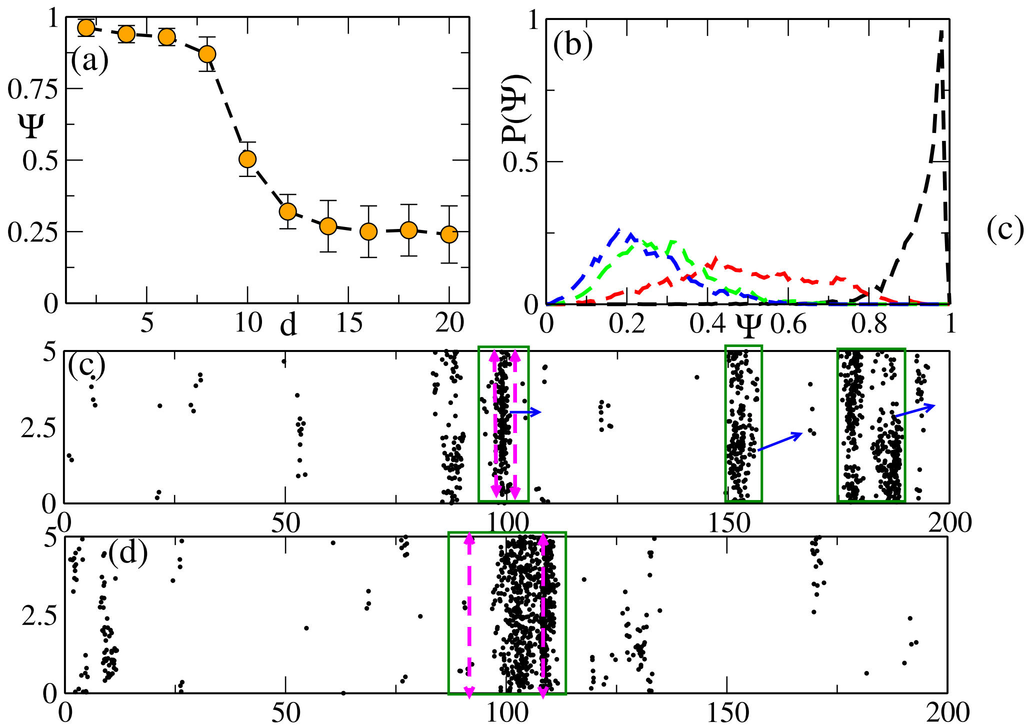

Fig. 5.3 (color online) All the plots (a)-(d) shown here for with perturbation. (a) We plot the global orientation order parameter Ψ vs. width of the disorder region *d* with perturbation. (b) Plot shows the global order parameter distribution $P(\Psi)$ for different width of the junction 'd'. Different colored break lines are for d=4 (black), d=8 (red), d=12 (green) and d=18 (green). Plot (c) and (d) show the space snapshots of the system for width d=2 and 18 respectively. Pink lines show the bounry of the junction and blue lines with arrow show the mean orientation of the local flock. $L \times W = 200 \times 5$ and $\rho = 1.0$

have found that global orientation order parameter Ψ decay sharply with an increase in the junction width 'd' shown in fig.5.3(a). Which has been confirmed by plotting orientation distribution $P(\Psi)$ for different junction width in fig.5.3(b). Further in fig.5.3(c)-(d) we plot the snapshots for different junction widths 'd=2 and 16'. For lower width of junction flock does not experience any hurdle and passes coherently with different bands, leads to higher values of Ψ. Moreover, for higher values of junction width, most of the SPPs trapped into the junction with random directions hence decreases in the value of Ψ. Further, we study the system without perturbation in the steady state.

Properties of flock at the junction

Study of junction current:- In this section, We discuss the junction current within the junction along the long x-axis as well as small the y-axis and, finally, the total current at the junction with the variation of the junction width d. The junction current is calculated when at least 25% particles of the whole system are within the junction, and we named this current as an event current. The event current in the junction along x and y-direction is defined by $\Psi_{xd} = \frac{1}{n}\sum_i^n v_{xi}$, $\Psi_{yd} = \frac{1}{n}\sum_i^n v_{yi}$ and finally total event current $\Psi_d(t) = \frac{1}{n}|\sum_i^n n_i(t)|$. where v_{xi}, v_{yi}, and n represent the components of velocity vector along the long and short

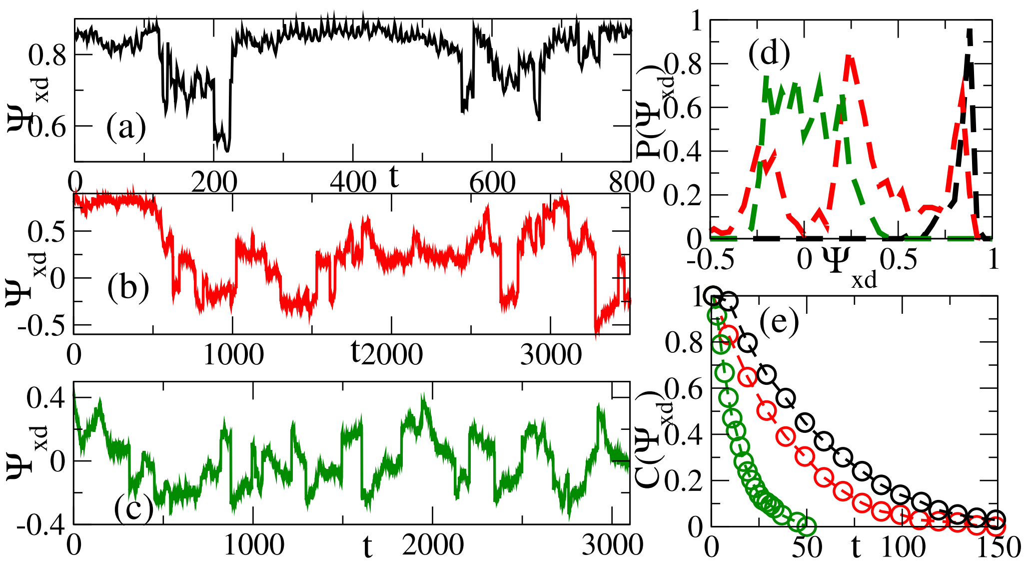

Fig. 5.4 (color online) Plot (a)-(show the time variation of event current Ψ_{xd} along the long axis with increasing width d. (d) event current distribution $P(\Psi_{xd})$. (e) Shows the x-orientation current autocorrelation for three junction width 'd'. Black, red and green colors show the results for junction width d=4,8 and 12 respectively. $L \times W = 200 \times 5$ and $\rho = 1.0$.

axis, and the total number of particles within the junction. In the fig. 5.4(a)-(c) We show the time series of Ψ_{xd} for different values of junction width d. We observe, with increased d, the amplitude of Ψ_{xd} decreases and also positive and negative current changes in a periodic fashion with the decreased period. Here current is carried by the particles along +ve and -ve x-direction, we call them positive and negative current. Consecutive the

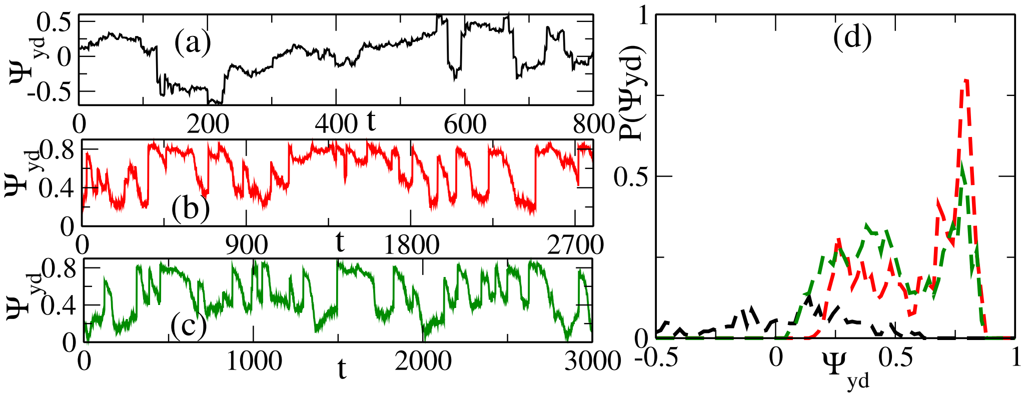

Fig. 5.5 (color online) Plot (a)-(c) show the time variation of orientation event current Ψ_{yd} along the long axis with increasing width d. (d) Orientation event current distribution $P(\Psi_{yd})$. Black, red and green colors show the junction width d=4,8 and 12 respectively. $L \times W = 200 \times 5$ and $\rho = 1.0$.

positive and negative peaks in the event current in x-direction correspond to the positive and negative currents along the long axis respectively. Further, in fig.5.4(d); we show the current distribution of Ψ_{xd} along the long direction which, clearly suggest that with the increase in the width of the junction, there is a clear signature of current reversal. Also, in fig.5.2(m) we plot the current-current autocorrelation $C(\Psi_{xd}) =< \Psi_{xd}(0) \cdot \Psi_{xd}(t) >$. Sharper decay of autocorrelation with the increase in the junction width 'd'. Sharper decay of $C(\Psi_{xd})$ which further confirm the frequent current reversal with the increase of the junction width. Furthermore, in fig.5.5(a)-(c), we show the junction current Ψ_{yd} and current distribution $P(\Psi_{yd})$ along the small axis with respect to junction width d. We observe that there is no current reversal with the increase in d. However, for higher d, there is a periodicity which is further confirmed by the current distribution $P(\Psi_{yd})$ is shown shown in fig.5.5(d). Finally, in the fig.5.6(a) we plot the global orientation order parameter $\Psi_d(t)$ and corresponding distribution $P(\Psi_d)$ with respect to the width of the junction d within the junction. Here Ψ_d vs. d, it is very clear that with the increase in the junction width (d), total event current (Ψ_d) decreases monotonically, which is further confirmed by $P(\Psi_d)$ vs. Ψ_d in fig.5.6(b).

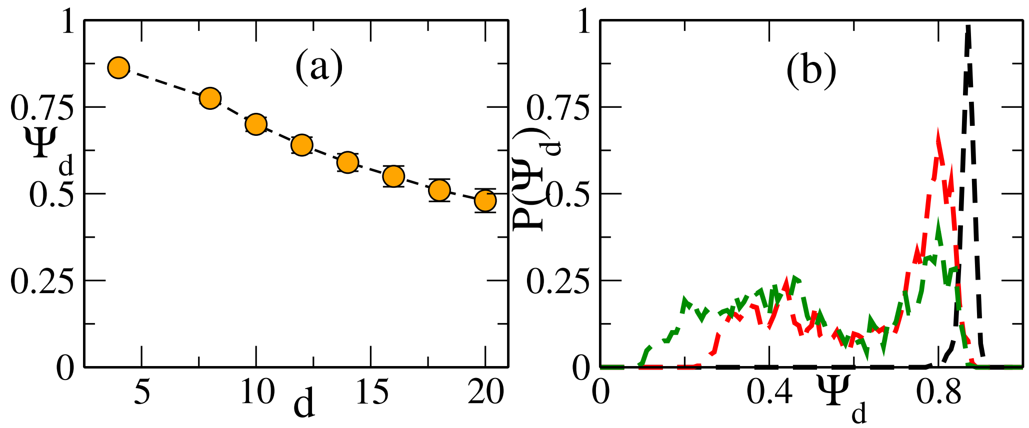

Fig. 5.6 (color online) Plot (a) show the global orientation order parameter Ψ_d with junction width 'd', and (b) show the probability distribution $P(\Psi_d)$ for junction width d=4 (black), 8 (red) and 12 (green) respectively. $L \times W = 200 \times 5$ and $\rho = 1.0$.

5.4 Summary and discussion

In this chapter, we have considered the flock of polar self-propelled particles moving on a two dimensional ractangular channel along an order-disorder interface with periodic boundary conditions. The intraction among the particles are taken as Vicsek type viz; particles move with constant speed and interact through short range alignment interaction. Inside the junction, particles experience a high noise disorder state, and outside they are in the ordered state. The width of the junction is adjusted by the junction width parameter 'd'. The model is motivated by the Josephson junction, an analogous equilibrium system. Interestingly, flock experience more disturbance for wider junction width in the system with perturbation in comparison to system without perturbation. Further, at the junction, we have found the current reversal for a critical width of the junction, which is a common feature of the Josephson junction. Further, the particle current at the junction decreases with an increase in the junction width.

Hence, this study can be useful to understand the active matter systems at the two different boundaries. It can help to answer the response of the flock to change in the external conditions along their move.

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