

# Project Presentation

Shaswata Roy

Indian Institute of Technology Madras

*under Prof. Neelima Gupte*

November 29, 2018

- 1 Recap of Vicsek Model
  - Recap
- 2 Analytical Models
  - Hydrodynamic Descriptions
- 3 Passive rods among Active Rods
  - Passive rods
  - Mixture
- 4 Ongoing and Future Work

# Recap

- Group of particles confined to a 2D box having equal speeds and whose angular position depends on it's neighbours.

# Recap

- Group of particles confined to a 2D box having equal speeds and whose angular position depends on it's neighbours.
- The equations of motion are given by,

$$\theta(t+1) = \langle \theta(t) \rangle_r + \xi(t) \quad \xi \in [-\eta/2, \eta/2] \quad (1)$$

$$x(t+1) = x(t) + v_0 \Delta t \quad (2)$$

# Recap

- Group of particles confined to a 2D box having equal speeds and whose angular position depends on it's neighbours.
- The equations of motion are given by,

$$\theta(t+1) = \langle \theta(t) \rangle_r + \xi(t) \quad \xi \in [-\eta/2, \eta/2] \quad (1)$$

$$x(t+1) = x(t) + v_0 \Delta t \quad (2)$$

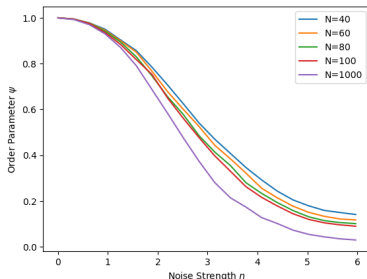


Figure: Original VM

- To describe the collective motion of rods we consider an interaction potential which penalizes the overlap of the rods.

- To describe the collective motion of rods we consider an interaction potential which penalizes the overlap of the rods.
- Overlapping area of the rods was proportional to  $-\cos^2(\theta_j - \theta_i)$  (Onsager)

- To describe the collective motion of rods we consider an interaction potential which penalizes the overlap of the rods.
- Overlapping area of the rods was proportional to  $-\cos^2(\theta_j - \theta_i)$  (Onsager)

$$U_i(x_i, \theta_i) = -\frac{\gamma}{2} \sum_{|x_i - x_j| < R} \cos(2(\theta_j - \theta_i))$$



- To describe the collective motion of rods we consider an interaction potential which penalizes the overlap of the rods.
- Overlapping area of the rods was proportional to  $-\cos^2(\theta_j - \theta_i)$  (Onsager)

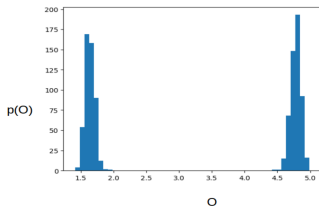
$$U_i(x_i, \theta_i) = -\frac{\gamma}{2} \sum_{|x_i - x_j| < R} \cos(2(\theta_j - \theta_i))$$

$$x_i = v_0 V(\theta_i)$$

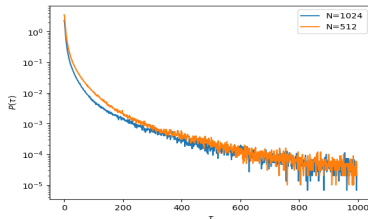
$$\dot{\theta}_i = \gamma \sum_{|x_i - x_j| < R} \sin(2(\theta_j - \theta_i)) + \xi_i(t)$$

- The probability of the order parameter has 2 peaks at a difference of  $\pi$  from each other.

- The probability of the order parameter has 2 peaks at a difference of  $\pi$  from each other.

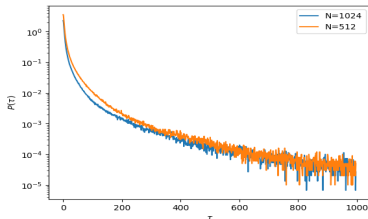
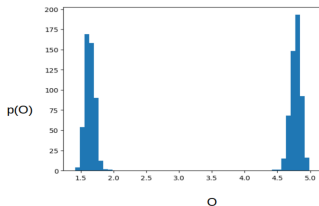


(c) Probability Order Parameter



(d) Probability of  $\tau$  distribution

- The probability of the order parameter has 2 peaks at a difference of  $\pi$  from each other.

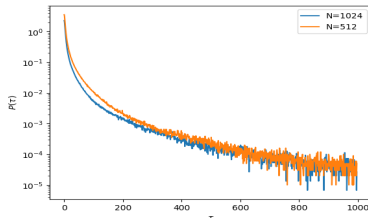
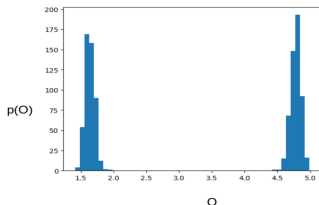


(e) Probability Order Parameter

(f) Probability of  $\tau$  distribution

- Polar Order:  $S_1 = \langle \exp i\theta(t) \rangle_t$  and nematic order:  $S_2 = \langle \exp 2i\theta(t) \rangle_t$

- The probability of the order parameter has 2 peaks at a difference of  $\pi$  from each other.



(g) Probability Order Parameter

(h) Probability of  $\tau$  distribution

- Polar Order:  $S_1 = \langle \exp i\theta(t) \rangle_t$  and nematic order:  $S_2 = \langle \exp 2i\theta(t) \rangle_t$
- Polar Order parameter is negligible.

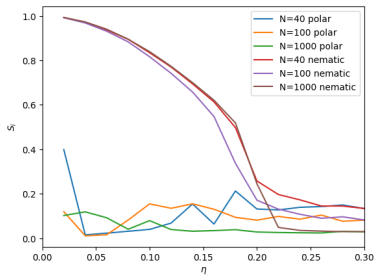


Figure: Order Parameters against Noise

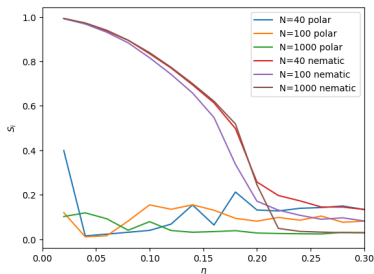


Figure: Order Parameters against Noise

- Nematic order undergoes a phase transition. However does not seem to follow a power law throughout.

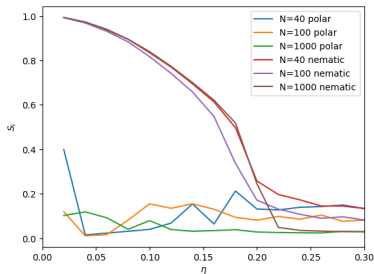


Figure: Order Parameters against Noise

- Nematic order undergoes a phase transition. However does not seem to follow a power law throughout.

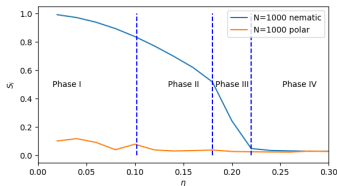


Figure: Phases



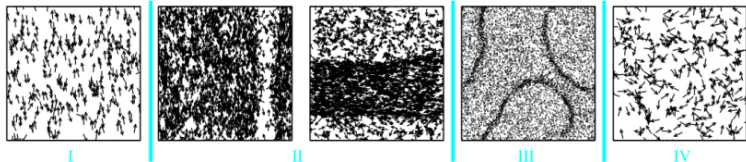


Figure: Order Parameters against Noise

# Hydrodynamic Descriptions

- A.Peshkov and group considered a dilute limit where only binary interactions take place. Assuming that the orientations are uncorrelated the Boltzmann equation governing the one particle distribution is given by,

$$\partial_t f(\vec{r}, \theta, t) + v_0 \vec{e}(\theta) \cdot \nabla f(\vec{r}, \theta, t) = I_{dif}[f] + I_{col}[f]$$

Where  $I_{dif}[f]$  is the self diffusion term and  $I_{col}[f]$  is the collision integral.

# Hydrodynamic Descriptions

- A.Peshkov and group considered a dilute limit where only binary interactions take place. Assuming that the orientations are uncorrelated the Boltzmann equation governing the one particle distribution is given by,

$$\partial_t f(\vec{r}, \theta, t) + v_0 \vec{e}(\theta) \cdot \nabla f(\vec{r}, \theta, t) = I_{dif}[f] + I_{col}[f]$$

Where  $I_{dif}[f]$  is the self diffusion term and  $I_{col}[f]$  is the collision integral.

- We see that

$$\rho(\vec{r}, t) = \int_{-\pi}^{\pi} d\theta f(\vec{r}, \theta, t)$$

$$\rho(\vec{r}, t) \vec{u}(\vec{r}, t) = \int_{-\pi}^{\pi} d\theta f(\vec{r}, \theta, t) \vec{e}(\theta)$$

# Hydrodynamic Descriptions

- A.Peshkov and group considered a dilute limit where only binary interactions take place. Assuming that the orientations are uncorrelated the Boltzmann equation governing the one particle distribution is given by,

$$\partial_t f(\vec{r}, \theta, t) + v_0 \vec{e}(\theta) \cdot \nabla f(\vec{r}, \theta, t) = I_{dif}[f] + I_{col}[f]$$

Where  $I_{dif}[f]$  is the self diffusion term and  $I_{col}[f]$  is the collision integral.

- We see that

$$\rho(\vec{r}, t) = \int_{-\pi}^{\pi} d\theta f(\vec{r}, \theta, t)$$

$$\rho(\vec{r}, t) \vec{u}(\vec{r}, t) = \int_{-\pi}^{\pi} d\theta f(\vec{r}, \theta, t) \vec{e}(\theta)$$

- Integrating over  $\theta$  would give us back the continuity equation.

# Fourier Expansion

- Fourier series expansion of  $f$  with respect to  $\theta$ ,

$$\hat{f}_k(\vec{r}, t) = \int_{-\pi}^{\pi} d\theta f(\vec{r}, \theta, t) \exp ik\theta$$

- Fourier series expansion of  $f$  with respect to  $\theta$ ,

$$\hat{f}_k(\vec{r}, t) = \int_{-\pi}^{\pi} d\theta f(\vec{r}, \theta, t) \exp ik\theta$$

- It can be seen now that  $\hat{f}_1(r, t)$  gives us the coarse grained approximation of the polar order parameter and  $\hat{f}_2(r, t)$  gives us the coarse grained approximation of the nematic order parameter

# Fourier Expansion

- Fourier series expansion of  $f$  with respect to  $\theta$ ,

$$\hat{f}_k(\vec{r}, t) = \int_{-\pi}^{\pi} d\theta f(\vec{r}, \theta, t) \exp ik\theta$$

- It can be seen now that  $\hat{f}_1(r, t)$  gives us the coarse grained approximation of the polar order parameter and  $\hat{f}_2(r, t)$  gives us the coarse grained approximation of the nematic order parameter
- $(\hat{f}_1, \hat{f}_2) = (0, \sqrt{\mu/\xi})$  which confirms that the polar order is always 0 while the nematic order undergoes a phase transition when  $\mu > 0$ .



$$x_i = \sigma_i(t)$$

$$\theta_i = \gamma \sum_{|x_i - x_j| < R} \sin(2(\theta_j - \theta_i)) + \xi_i(t)$$





$$x_i = \sigma_i(t)$$

$$\theta_i = \gamma \sum_{|x_i - x_j| < R} \sin(2(\theta_j - \theta_i)) + \xi_i(t)$$

- Here  $\sigma_i(t)$  is an isotropic delta-correlated vectorial noise.



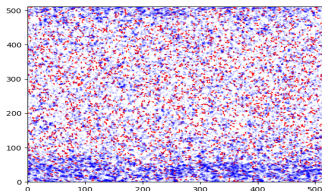
$$x_i = \sigma_i(t)$$

$$\dot{\theta}_i = \gamma \sum_{|x_i - x_j| < R} \sin(2(\theta_j - \theta_i)) + \xi_i(t)$$

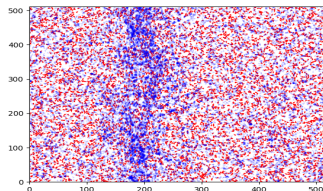
- Here  $\sigma_i(t)$  is an isotropic delta-correlated vectorial noise.
- System of passive rods evolving according to the above equations exhibits QLRO (decays with system size).

# Mixture

- We introduce passive rods in dilute amounts in a system of active rods.



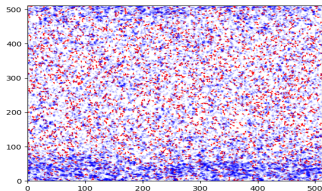
(a) Passive Rods (10%)



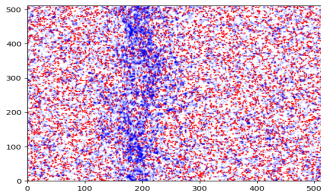
(b) [Passive Rods (20%)

# Mixture

- We introduce passive rods in dilute amounts in a system of active rods.



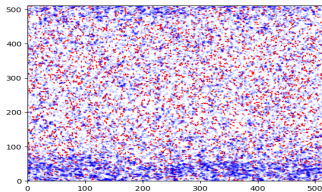
(c) Passive Rods (10%)



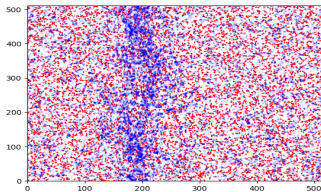
(d) [Passive Rods (20%)

# Mixture

- We introduce passive rods in dilute amounts in a system of active rods.



(e) Passive Rods (10%)



(f) [Passive Rods (20%)

- The band structure exists even though the active and passive rods interact among each other. However the band structure completely disappears when we consider a smaller system size.

# Mixture

- Possible reason could be the low density of the bands in smaller system size.

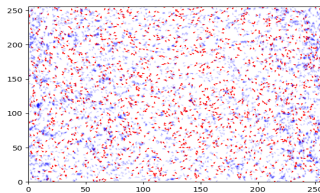


Figure: Smaller System Mixture

# Mixture

- Possible reason could be the low density of the bands in smaller system size.

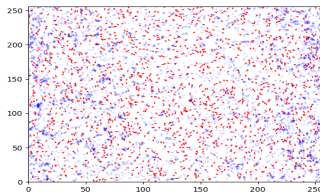


Figure: Smaller System Mixture

- The passive rods and the active rods seem to exhibit similar phase plots when plotted as it would independently.

# Mixture

- Possible reason could be the low density of the bands in smaller system size.

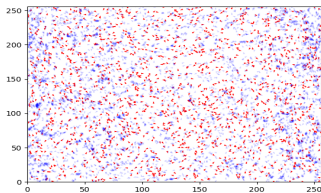
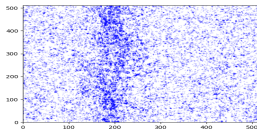
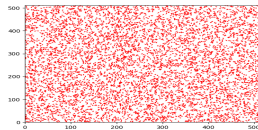


Figure: Smaller System Mixture

- The passive rods and the active rods seem to exhibit similar phase plots when plotted as it would independently.



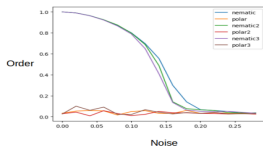
(a) Active Rods



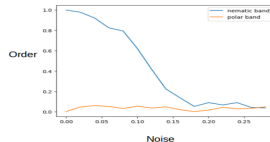
(b) Passive Rods



- However there is a small change when we compare the phase transitions at different dilutions.

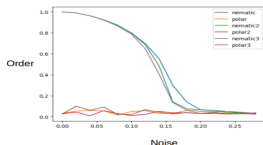


(c) Mixture Phase Transition

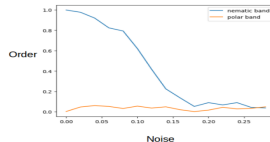


(d) Passive particles phase transition

- However there is a small change when we compare the phase transitions at different dilutions.



(e) Mixture Phase Transition



(f) Passive particles phase transition

- There is a small decrease in the critical noise of phase transition. Furthermore there seems to be a phase transition in the passive particles as well which is probably induced by the interactions with the active rods.

# Ongoing and Future Works

## Volume Exclusion Effects

Steric Effects have only been considered in the angular orientation till now. By considering a potential penalizing the overlap in the translation term as well we can get a much more exact model.

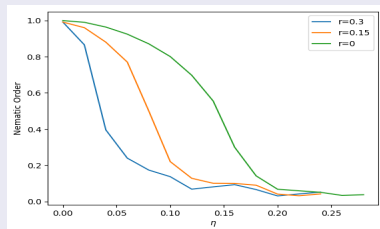


Figure: Effects of Size

## Kihara Potential

$$\Phi(r) = \Phi_0 \left( \frac{m}{n-m} \left( \frac{\rho_0}{\rho} \right)^n - \frac{n}{n-m} \left( \frac{\rho_0}{\rho} \right)^m \right)$$

## Formation of Band like structures

High density nematic bands are formed only when the size of the system is greater than  $\lambda_C$ . They are also formed in at specific noise strengths. The occurrence of these bands is poorly understood.

- F. Peruani, Active Brownian Rods
- E. Bertin, Michel Droz, Guillaume Gregoire, Boltzmann and hydrodynamic description for self propelled rods
- T. Vicsek, A. Czirok, E. Ben-Jacob, I. Cohen Novel Phase Transitions in Self Driven Systems, P