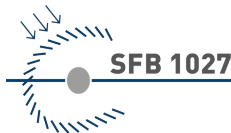




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POLAR FLOCKS WITH DISCRETIZED DIRECTIONS: THE ACTIVE CLOCK MODEL APPROACHING THE VICSEK MODEL

M. MANGEAT¹, S. CHATTERJEE¹, AND H. RIEGER^{1,2}

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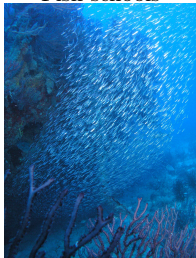
MONDAY, MARCH 27th

DPG Meeting - Dresden 2023 (DY 10.2)

- 1 Introduction on collective motions
- 2 Different theoretical flocking models
- 3 Active clock model
- 4 Conclusion

Natural and artificial collective motions

Fish schools



Becco et al., Physica
A (2006)

Bird flocks

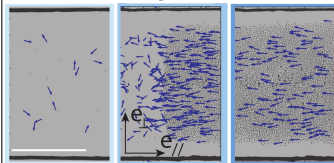


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Ballerini et al., PNAS (2008)

bacteria swarm, human crowds, ...

Rolling colloids

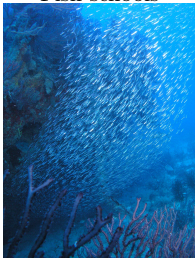


Bricard et al., Nature (2013)

liquid droplets, vibrating polar
disks, ...

Natural and artificial collective motions

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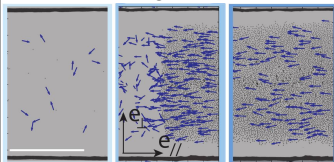


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How to create a collective motion?

- ▶ Out-of-equilibrium phenomenon: active matter system with a large number of particles:
 - ▶ consuming internal energy to self-propel,
 - ▶ interacting via alignment and/or repulsion.
- ▶ Flocking transition: spontaneous synchronized motion of large clusters (*flocks*) emerges for large densities and/or low noise.

First theoretical model (2D): The Vicsek model (1995)

- ▶ Self-propelled particles with constant speed, aligning in the local average direction.

$$\theta_i(t+1) = \langle \theta(t) \rangle_r + \eta \xi_i(t)$$

$$\mathbf{x}_i(t+1) = \mathbf{x}_i(t) + v \mathbf{e}_i(t+1)$$

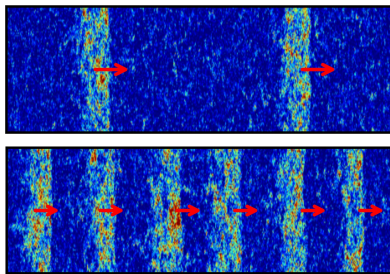
with $\mathbf{e}_i(t+1)$ in the direction of $\theta_i(t+1)$ and $\xi_i(t)$ a random number in $[-\pi, \pi]$.

- ▶ Ferromagnetic interactions where η plays the role of the temperature.

T. Vicsek et al., Phys. Rev. Lett. **75**, 1226 (1995)

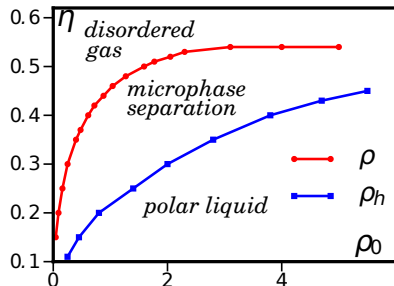
- ▶ Hydrodynamic limit belongs to universality class of the XY model.

J. Toner and Y. Tu, Phys. Rev. Lett. **75**, 4326 (1995)



- ▶ Spontaneous breaking of the continuous symmetry.
- ▶ First-order liquid-gas phase transition, with microphase separation.

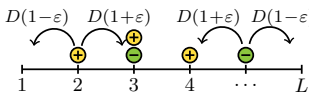
A. P. Solon et al., Phys. Rev. Lett. **114**, 068101 (2015)



The active Ising model (AIM)

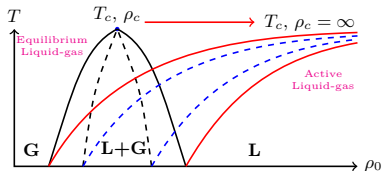
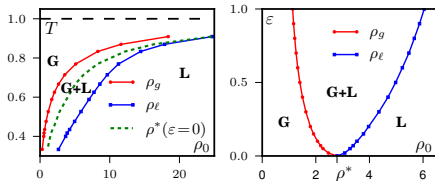
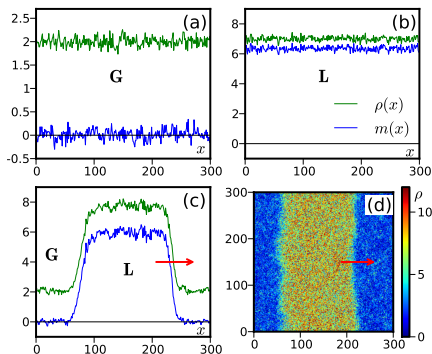
Biased Diffusion

Spin Flips



$$W_{\text{hop}} = D(1 \pm \epsilon)$$

$$W_{\text{flip}}(\sigma \rightarrow -\sigma) = \gamma \exp(-\beta\sigma m_i/\rho_i)$$



- The flocking transition is a first-order liquid-gas phase transition, without the supercritical region ($T_c = 1$).

 A. P. Solon and J. Tailleur, Phys. Rev. Lett. **111**, 078101 (2013)

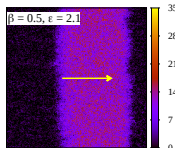
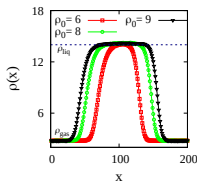
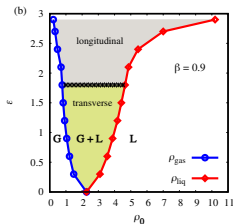
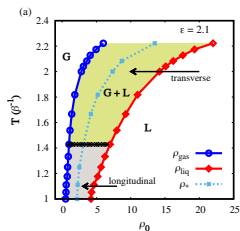
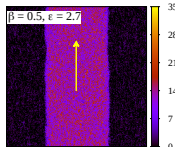
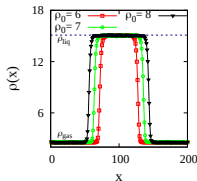
 A. P. Solon and J. Tailleur, Phys. Rev. E **92**, 042119 (2015)

The q -state active Potts model (APM) [$q = 4$ and $q = 6$]

- ▶ Hopping rate in preferred direction: $D(1 + \varepsilon)$ and in other directions: $D[1 - \varepsilon/(q - 1)]$.
- ▶ Local Hamiltonian and flipping rate on site i :

$$H_i^{\text{APM}} = -\frac{J}{2\rho_i} \sum_{k=1}^{\rho_i} \sum_{l \neq k} (q\delta_{\sigma_i^k, \sigma_i^l} - 1), \quad W_{\text{flip}}(\sigma \rightarrow \sigma') \propto \exp(-\beta\Delta H_i^{\text{APM}}).$$

- ▶ Reorientation transition: transverse bands (small ε) to longitudinal lanes (large ε).
- ▶ Flocking transition is a first-order liquid-gas phase transition.

 $t = 10^5$

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 S. Chatterjee, M. Mangeat, R. Paul, and H. Rieger, EPL **130**, 66001 (2020)

 M. Mangeat, S. Chatterjee, R. Paul, and H. Rieger, Phys. Rev. E **102**, 042601 (2020)

The q -state active clock model (ACM)

- ▶ Motivation: investigate the $q \rightarrow +\infty$ limit and see if the VM is recovered:
 - ▶ microphase separation in the coexistence phase,
 - ▶ absence of the reorientation transition,
 - ▶ quasi-long range order (QLRO) at $v \rightarrow 0$ limit.

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- ▶ N particles in a **off-lattice $L_x \times L_y$ rectangular domain**. Average density: $\rho_0 = N/L_x L_y$.
- ▶ i th particle characterized by position \mathbf{x}_i and orientation $\theta_i \in \{0, 2\pi/q, \dots, 2\pi(q-1)/q\}$.
- ▶ Neighborhood $\mathcal{N}_i = \{j \text{ with } |\mathbf{x}_i - \mathbf{x}_j| < 1\}$ of i th particle, constituted of ρ_i particles.
- ▶ Local clock Hamiltonian and local magnetization in the neighborhood \mathcal{N}_i :

$$H_i^{\text{ACM}} = -\frac{J}{2\rho_i} \sum_{k \in \mathcal{N}_i} \sum_{\substack{l \in \mathcal{N}_i \\ l \neq k}} \cos(\theta_l - \theta_k), \quad \mathbf{m}_i = \sum_{k \in \mathcal{N}_i} (\cos \theta_k, \sin \theta_k).$$

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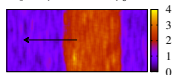
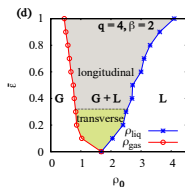
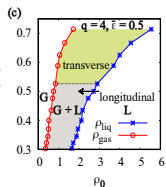
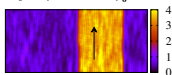
$$H_i^{\text{ACM}} = -\frac{J}{2\rho_i} \sum_{k \in \mathcal{N}_i} \sum_{\substack{l \in \mathcal{N}_i \\ l \neq k}} \cos(\theta_l - \theta_k), \quad \mathbf{m}_i = \sum_{k \in \mathcal{N}_i} (\cos \theta_k, \sin \theta_k).$$

- ▶ At each time t , the i th particle in state $\theta_i = \theta$ can
 - ▶ hop in preferred direction $\phi = \theta$ with a rate: $D(1 + \varepsilon)$,
 - ▶ hop in another direction $\phi \neq \theta$ with a rate: $D[1 - \varepsilon/(q-1)]$,
 - ▶ flip to an orientation $\theta' \neq \theta$, for a temperature $T = \beta^{-1}$, with a rate:

$$W_{\text{flip}}(\theta \rightarrow \theta') = \gamma \exp(-\beta \Delta H_i^{\text{ACM}}) = \gamma \exp \left\{ \frac{\beta J}{\rho_i} [\mathbf{m}_i \cdot (\mathbf{e}_{\theta'} - \mathbf{e}_\theta) + 1 - \cos(\theta' - \theta)] \right\}.$$

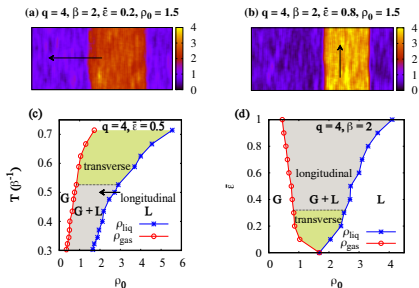
- ▶ Rescaled quantities (for an infinite q limit well-defined):

$$\bar{D} = qD \quad \text{and} \quad \bar{\varepsilon} = \frac{\varepsilon}{q-1}.$$

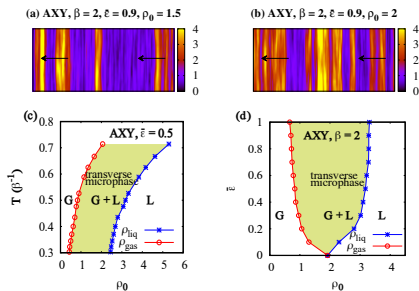
Results for $q = 4$ and $q = \infty$ $q = 4$ -state active clock model(a) $q = 4, \beta = 2, \tilde{\varepsilon} = 0.2, \rho_0 = 1.5$ (b) $q = 4, \beta = 2, \tilde{\varepsilon} = 0.8, \rho_0 = 1.5$ 

- ▶ Liquid-gas phase transition, with macrophase separation in the coexistence region (like AIM and APM).
- ▶ Presence of the reorientation transition (like APM), from transverse band (low bias ε) to longitudinal lane (high bias ε).

S. Chatterjee, M. Mangeat, and H. Rieger, EPL **138**, 41001 (2022)

Results for $q = 4$ and $q = \infty$ $q = 4$ -state active clock model

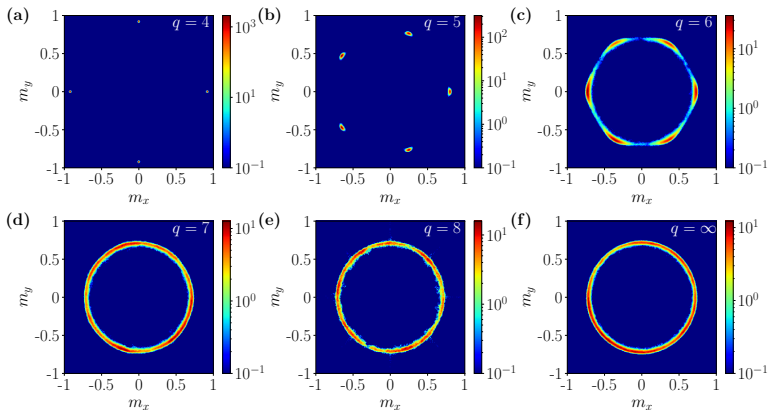
- ▶ Liquid-gas phase transition, with macrophase separation in the coexistence region (like AIM and APM).
- ▶ Presence of the reorientation transition (like APM), from transverse band (low bias ε) to longitudinal lane (high bias ε).

active XY model ($q = \infty$)

- ▶ Liquid-gas phase transition, with microphase separation in the coexistence region (like VM).
- ▶ Absence of the reorientation transition (only transverse bands are observed).

q -dependence on the ordered phase without activity ($\varepsilon = 0$)

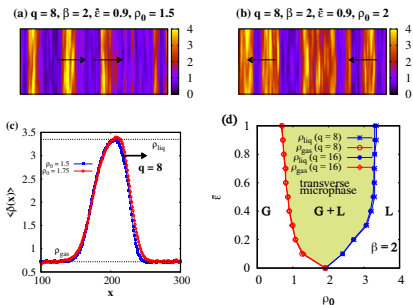
- Magnetization distribution for $\beta = 2$, $\rho_0 = 3$, in 50×50 domain.



- For $q \leq 5$: “pinned” orientations (LRO), and for $q \geq 6$: “unpinned” orientations (QLRO).
- The transition QLRO/LRO may depend on temperature, density and system size.

Results for finite q values

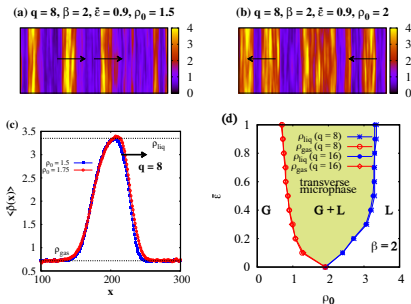
Coexistence phase and phase diagram



- ▶ Liquid-gas phase transition, with microphase separation in the coexistence region (like VM).
- ▶ Absence of the reorientation transition.

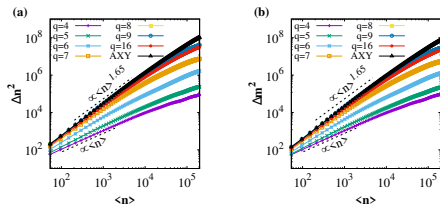
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Coexistence phase and phase diagram



- ▶ Liquid-gas phase transition, with microphase separation in the coexistence region (like VM).
- ▶ Absence of the reorientation transition.

Number and magnetization fluctuations in liquid phase



- ▶ $\Delta n^2 \sim \langle n \rangle^\xi$ and $\Delta m^2 \sim \langle n \rangle^\xi$, with

q	4	5	6	7	8	∞
ξ	1.04	1.08	1.36	1.56	1.62	1.65

- ▶ macrophase separation $\Rightarrow \xi = 1$, normal fluctuations ($q \leq 5$).
- ▶ microphase separation $\Rightarrow \xi > 1$, giant fluctuations ($q \geq 6$).
- ▶ No asymptotic regime at large $\langle n \rangle$ observed for our system sizes ($L_x = L_y \leq 800$).

Hydrodynamic description

- Hydrodynamic equations for the density $\rho(\mathbf{x}; t)$ and the magnetization $\mathbf{m}(\mathbf{x}; t)$:

$$\begin{aligned}\partial_t \rho &= D_0 \nabla^2 \rho + \frac{v}{4} \nabla \cdot (\nabla \cdot Q) - v \nabla \cdot \mathbf{m}, \\ \partial_t \mathbf{m} &= D_0 \nabla^2 \mathbf{m} + \frac{v}{8} \begin{pmatrix} \partial_{xx} - \partial_{yy} & 2\partial_{xy} \\ 2\partial_{xy} & -\partial_{xx} + \partial_{yy} \end{pmatrix} \mathbf{m} - \frac{v}{2} (\nabla \rho + \nabla \cdot Q) \\ &\quad + \gamma_0 \left[\beta J - 1 - \frac{r}{\rho^{2-\xi}} - \kappa \frac{\mathbf{m}^2}{\rho^2} \right] \mathbf{m}.\end{aligned}$$

with diffusion constant: $D_0 = \overline{D}/4$, self-propulsion velocity: $v = \overline{D}\overline{\varepsilon}$, ferromagnetic interaction strength $\gamma_0 = q\gamma/(q-1)$, $\kappa = (\beta J)^2(7-3\beta J)/8$, and nematic tensor

$$Q = \frac{\beta J}{2\rho} \begin{pmatrix} m_x^2 - m_y^2 & 2m_x m_y \\ 2m_x m_y & -m_x^2 + m_y^2 \end{pmatrix}.$$

- Impossible to conclude about macrophase/microphase separation in the coexistence region with vectorial PDEs [Solon *et al.*, PRL **114**, 068101 (2015)]. We need to introduce a noise term (future work).

S. Chatterjee, M. Mangeat, and H. Rieger, EPL **138**, 41001 (2022)

Conclusion

- ▶ For the $q = 4$ -state ACM, we recover the same properties as the AIM and the APM: macrophase separation, presence of the reorientation transition, and LRO phase.
- ▶ For the AXYM ($q = \infty$), we recover the same properties as the VM: microphase separation, absence of the reorientation transition, and QLRO phase.
- ▶ For other q values (at fixed $\beta = 2$ and $\bar{\varepsilon} = 0.9$, with $L \leq 800$): we observe macrophase separation for $q \leq 5$, and microphase separation for $q \geq 6$, as well as a QLRO/LRO transition at $\varepsilon = 0$.

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Open questions and perspectives

- ▶ Do the number fluctuations in the liquid phase have an impact on the coexistence phase?
- ▶ Are the pinned/unpinned orientations in liquid phase equivalent to macrophase/microphase separation in coexistence region?
- ▶ Are the pinned/unpinned orientations equivalent to normal/giant number fluctuations in liquid phase?
- ▶ Many differences observed compared to the study made by Solon *et al.* [PRL **128**, 208004 (2022)], for a slightly different model (different hopping/flipping rates). From where these differences arise?
- ▶ Work on the hydrodynamic description to validate the simulation's results.

Thank you for your attention !

Following presentations

- ▶ Tuesday 28 at 12:00 PM: S. Chatterjee *et al.*, Flocking of unfriendly species: The two-species Vicsek model (BP 9.10 / TOE 317).
- ▶ Wednesday 29 at 03:45 PM: T. Guérin *et al.*, How stickiness can speed up diffusion in confined systems (DY 32.4 / ZEU 160).
- ▶ Thursday 30 at 01:00 PM: M. Mangeat *et al.*, Wetting of reflecting plates by an active Brownian fluid (DY 42.10 / P1).

References

- ▶ S. Chatterjee, M. Mangeat, R. Paul, and H. Rieger, *Flocking and reorientation transition in the 4-state active Potts model*, EPL **130**, 66001 (2020).
- ▶ M. Mangeat, S. Chatterjee, R. Paul, and H. Rieger, *Flocking with a q-fold discrete symmetry: Band-to-lane transition in the active Potts model*, Phys. Rev. E **102**, 042601 (2020).
- ▶ S. Chatterjee, M. Mangeat, and H. Rieger, *Polar flocks with discretized directions: the active clock model approaching the Vicsek model*, EPL **138**, 41001 (2022).