Scaling limits and behavior for microscopic stochastic models of active matter

based on JW with T. Bodineau, M. Kourbane-Houssène and J. Tailleur

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Active Matter

System composed of self-propelled individuals, maintaining itself out of equilibrium by *individual energy consumption*.

Rich phenomenology for active matter models :

$\rightarrow$ *Alignment phase transition*, between local alignment and global collective motion as the alignment strength increases.

$\rightarrow$ *Motility Induced Phase Separation (MIPS)*, dense clustering resulting from a slow down of particles in crowded regions.

Alignment phase transition

A local alignment mechanism between particle's velocities can result in long range ordering if the alignment noise is low enough.

Initially discovered by Vicsek at al. (1995), since then evidenced across many types of alignment mechanisms.

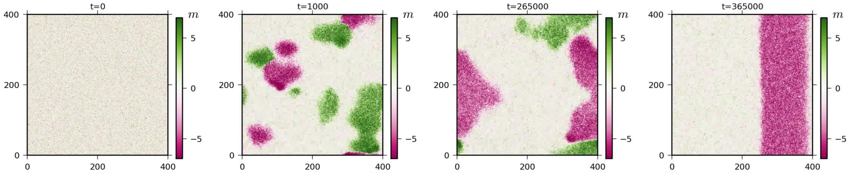


Figure: From *Flocking with discrete symmetry, the 2d active Ising model*, Solon & Tailleur 2015.

Mathematical derivation

Significant litterature in analysis, PDE and SPDEs, based on *mean-field interactions* :

$\mapsto$ Each particle interacts with a large number of neighbors

- *Continuum limit of self-driven particles with orientation interaction*, Degond, Motsch, 2007.
- *Mean field limit for the stochastic Vicsek's model*, Bolley, Carrillo, Canizo, 2011.
- Review on collective motion : *Macroscopic models of collective motion and self organization, review*, Degond & al., 2012

Motility Induced Phase Separation (MIPS)

Due to the positive feedback, particles cluster where they move slower, resulting in spontaneous condensation.

- MIPS can occur when the particle's velocity depends on the local density
- MIPS usually does not occur in models with alignment

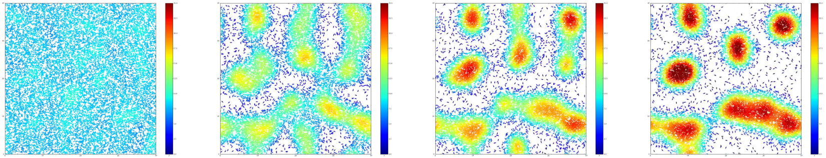


Figure: Coarsening effect in active matter. From Cates & Tailleur 2012.

Question : can these phenomena be rigorously derived starting from stochastic particle systems with local (microscopic range) interactions ?

$\mapsto$ **First simplification** : considering lattice gases, where particle hop randomly on a square lattice. The "velocity" of the particle is then represented by a drift in its jump rates

$\mapsto$ **Second simplification** : considering models with a couple of possible "velocities", i.e. particle types : in dimension 1 for example, "+" particles drifting right and "-" particles drifting left.

First try : Active Exclusion Process

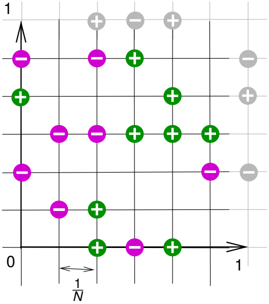
Two types of particles ($+$ and $-$) evolve on the **periodic square lattice** $\mathbb{T}_N^2 = \left\{0, \frac{1}{N}, \ldots, \frac{N-1}{N}\right\}^2$

For each site $x \in \mathbb{T}_N^2$, we define $\eta_x \in \{-1, 0, 1\}$.

$\mapsto \eta_x := \eta_x^+ - \eta_x^- = 0$, empty site

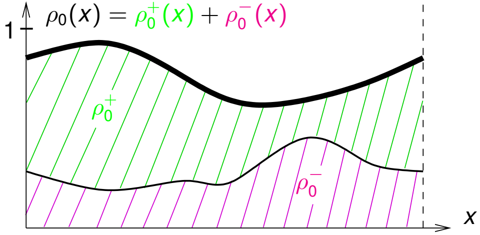
$\mapsto \eta_x^+ = 1$, $\eta_x^- = 0$ for a site occupied by ⊕.

$\mapsto \eta_x^- = 1$, $\eta_x^+ = 0$ for a site occupied by ⊖.



Initial configuration

- **Initial macroscopic smooth profiles** ρ_0^+ and ρ_0^-, $[0,1]^2 \to [0,1]$.
- $\rho_0 = \rho_0^+ + \rho_0^-$ is the initial particle density



- Initial ***local equilibrium*** : independently for any $x \in \mathbb{T}_N^2$

$$\eta_x(0) = \begin{cases} \pm 1 & \text{w.p. } \rho_0^\pm(x) \\ 0 & \text{w.p. } 1 - \rho_0^+(x) - \rho_0^-(x) \end{cases}$$

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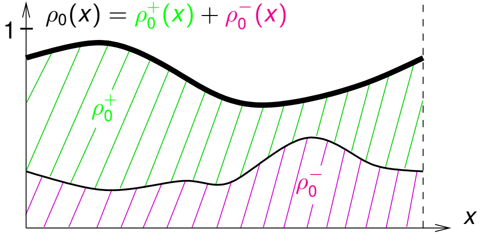

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The dynamics

Three parts to the dynamics :

- **Symmetric jumps with exclusion** : any particle ⊕/⊖ hops from site x to an *empty* neighboring site $x+z$ at rate N^2.
- **Weak asymmetric jumps with exclusion** : a particle ⊕ at site x hops at an extra rate λN to site $x+e_1$ *if it is empty*. A particle ⊖ at site x hops at an extra rate λN to site $x-e_1$ *if it is empty*.
- **Glauber dynamics** : a particle changes type at rate $e^{-\beta \sum_{|z|=1} \eta_x \eta_{x+z}}$

The parameters λ, β allow to tune the asymmetry and the alignment strength. Because of the different scaling in N, the three parts of the dynamics appear in the hydrodynamic limit.

Characterization of the macroscopic evolution

Weak formulation of the macroscopic evolution

The macroscopic ($N \to \infty$) state of the system is characterized by two macroscopic densities $\rho^+, \rho^- : [0, T] \times [0, 1]^2 \to [0, 1]$, where for any smooth function H,

$$\frac{1}{N^2} \sum_{x \in \mathbb{T}_N^2} H(x) \eta_x^+(t) \underset{N \to \infty}{\longrightarrow} \int_{[0,1]^2} dx H(x) \rho^+(t, x)$$

and

$$\frac{1}{N^2} \sum_{x \in \mathbb{T}_N^2} H(x) \eta_x^-(t) \underset{N \to \infty}{\longrightarrow} \int_{[0,1]^2} dx H(x) \rho^-(t, x).$$

Theorem (Hydrodynamic limit, E' 2021)

Assumption : $\forall u \in [0,1]^2$, $\rho_0(u) = \rho_0^+(u) + \rho_0^-(u) < 1$.

*The **macroscopic density** of particles $+$, denoted $\rho^+(t,u)$, is solution **in a weak sense** of the reaction-diffusion equation*

$$\partial_t \rho^+ = \nabla.\left[d_s(\rho)\nabla\rho^+ + D(\rho^+,\rho)\nabla\rho\right] + 2\widehat{\lambda}\partial_{x_1}\sigma(\rho^+,\rho) + \Gamma_\beta(\rho^+,\rho),$$

$$\rho^+(0,u) = \rho_0^+(u).$$

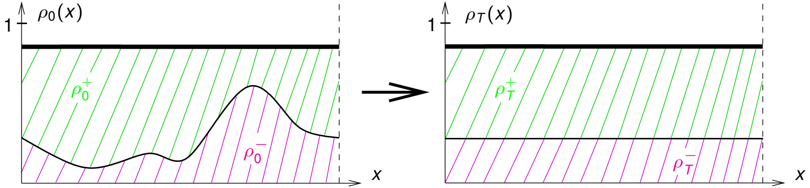
An analogous equation is verified by the $-$ particle density ρ^-, and $\rho = \rho^+ + \rho^-$ is the total particle density.

C. Kipnis and C. Landim.
Scaling limits of interacting particle systems.

J. Quastel.
Diffusion of colour in the simple exclusion process.

Dynamical interpretation

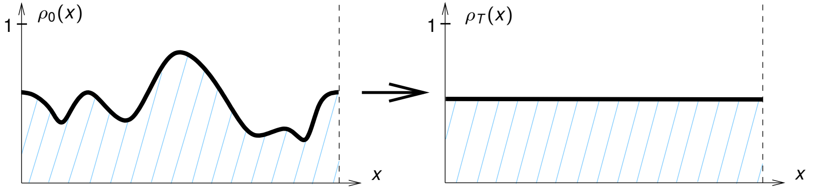
$$\partial_t \rho^+ = \nabla . \left[d_s(\rho) \nabla \rho^+ + D(\rho^+, \rho) \nabla \rho \right] + 2\widehat{\lambda} \partial_{x_1} \sigma(\rho^+, \rho) + \Gamma_\beta(\rho^+, \rho).$$



d_s is the ***self-diffusion coefficient*** of a tracer particle in an homogeneous environment.

Dynamical interpretation

$$\partial_t \rho^+ = \nabla . \Big[d_s(\rho) \nabla \rho^+ + D(\rho^+, \rho) \nabla \rho \Big] + 2\widehat{\lambda} \partial_{x_1} \sigma(\rho^+, \rho) + \Gamma_\beta(\rho^+, \rho).$$



The coefficient D quantifies the **diffusion** due to heterogeneities of the **total particle density**

$$D(\rho^+, \rho) = \frac{\rho^+}{\rho}(1 - d_s(\rho)) \quad \text{(Quastel, 1992).}$$

Remarks / issues

- The Einstein relation between D, d_s and σ is satisfied *in a matrix form*
- The assumption on the total density is required because of the lack of ergodicity of the jump dynamics at high densities
- The model is *non-gradient*, which induces significant mathematical difficulties. As a consequence, the diffusion and conductivity coefficients are *not explicit*, which is problematic to simulate and understand the behavior of the macroscopic model.

A simple 1-D model for MIPS

We change the model to try and make it more tractable, in order to be able to prove MIPS, starting from the microscopic model :

- **Symmetric jumps with swap** : the content of two neighboring sites is **swapped** at rate DN^2, regardless of whether or not they are empty or occupied.
- **Weak asymmetric jumps with exclusion** : a particle $\oplus$ at site x hops at an extra rate λN to site $x + e_1$ *if it is empty*. A particle $\ominus$ at site x hops at an extra rate λN to site $x - e_1$ *if it is empty*.
- **Glauber dynamics** : a particle changes type at constant rate $\gamma > 0$.

Because we allow neighboring particles to swap, the system becomes *gradient* and no longer has ergodicity issues at high densities.

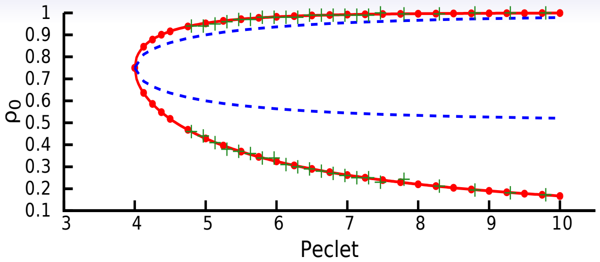
Given the macroscopic densities $\rho^{\pm}$ of particles ⊕ and ⊖, we consider the total density $\rho = \rho^+ + \rho^-$ and the local magnetization $m = \rho^+ - \rho^-$.

Theorem (Kourbane-Houssène, E', Bodineau, Tailleur 2018)

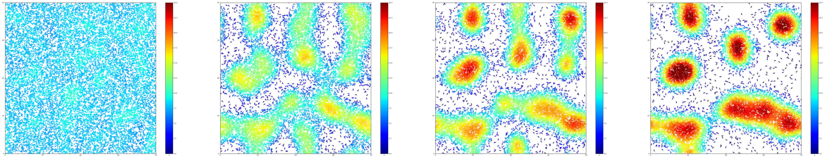
The macroscopic density and magnetization fields are solution to the system

$$\partial_t \rho = D\Delta\rho - \lambda\nabla m(1-\rho)$$
$$\partial_t m = D\Delta m - \lambda\nabla\rho(1-\rho) - 2\gamma m$$

From this explicit equation, an exact phase diagram can be obtained for MIPS, and the coexisting densities can be obtained analytically as a function of the Péclet number $Pe = \lambda/\sqrt{D\gamma}$



- Outside the spinodals (dashed blue), the uniform profile $\rho \equiv \rho_0$, $m \equiv 0$ is linearly stable.
- Inside the spinodals ultimately form two phases, a dense "liquid" phase and a "gaseous" phase with resp. densities given by the top and bottom red curves.



A 1-D zero-range alignment model

- **Symmetric jumps, no exclusion** : any particle jumps to each of its two neighbors at rate DN^2 (several particles can occupy the same site).

- **Weak asymmetric jumps, no exclusion** : a particle $\oplus$ (resp. $\ominus$) at site x jumps at an extra rate λN to site $x+1$ (resp $x-1$).

- **Glauber dynamics** : a particle $\oplus$ (resp. $\ominus$) at site x becomes $\ominus$ (resp. $\oplus$) at rate $e^{-\beta(\eta_x^+ - \eta_x^-)}$ (resp. $e^{\beta(\eta_x^+ - \eta_x^-)}$).

$\mapsto$ particles align their spin with other particles on the same site.

Theorem (Kourbane-Houssène, E', Bodineau, Tailleur 2018)

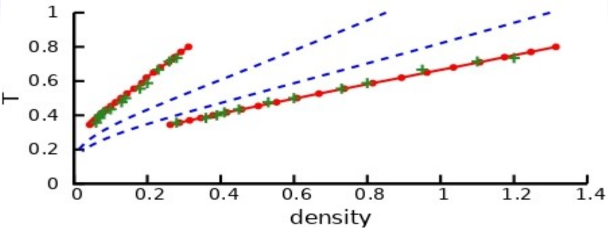
The macroscopic density and magnetization fields are solution to the system

$$\partial_t \rho = D\Delta\rho + \lambda\nabla m$$
$$\partial_t m = D\Delta m + \lambda\nabla\rho - F_\beta(\rho, m)$$

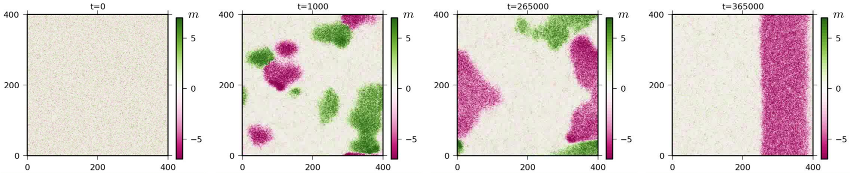
where F_β is explicit,

$$F_\beta(\rho, m) = 2\big[m\,\mathrm{ch}(m\sin\beta) - \rho\,\mathrm{sh}(m\,\mathrm{sh}\,\beta)\big]\,e^{-\beta+\rho\,\mathrm{ch}\,\beta-\rho}.$$

The homogeneous, non-magnetized solution $\rho \equiv \rho_0$, $m \equiv 0$ is linearly stable unless $\partial_m F_\beta(\rho, 0) < 0$. Once again, an exact phase diagram can be obtained for the alignment phase transition.



- Below the lower spinodal, $\rho \equiv \rho_0$, $m \equiv 0$ linearly stable.
- Above the upper spinodal, $\rho \equiv \rho_0$, $m \equiv m_0(\rho_0)$ linearly stable.
- Between the two spinodals, $\rho \equiv \rho_0$, $m \equiv m_0(\rho_0)$ is unstable, $\Longrightarrow$ travelling magnetized band, at density ρ_ℓ (right red curve) in a gaseous phase at density ρ_g (left red curve).



Projects and open questions

- *Ongoing with T. Bodineau* : degenerate exclusion model showing in some parameter regime a negative diffusion coefficient, which would be a tractable dynamical model for MIPS.
- To understand the emergence and selection of the metastable states, one needs to understand the finite scale fluctuations around the the hydrodynamic limit.
- Similarly, obtaining large deviation estimates (following Bertini and al.'s *macroscopic fluctuation theory*), would help to understand more qualitatively and quantitatively the dynamic aspects of theses phenomena.

Thanks for your attention !