Active matter and hydrodynamic limit for a collective dynamics model

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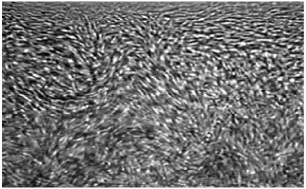
CAKE seminar, Cambridge
May 25th 2016

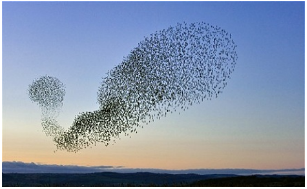
Plan of the talk

Plan of the talk

Collective motion & Active matter

Collective behavior can be observed among numerous animal species

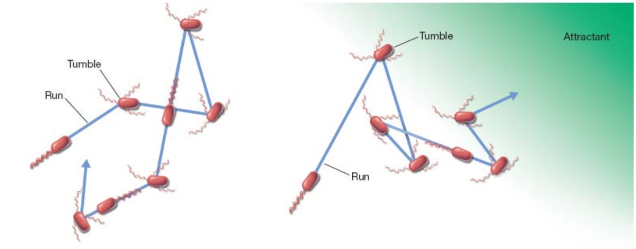





→ Classical representation : *Individual Based Models* (IBM) built around *active matter*.

Active Matter

System composed of many individuals, maintained out of equilibrium by an *energy influx at the individual level*.



(a) No attractant present: Random movement (b) Attractant present: Directed movement

Two types of phenomena can arise in active matter models :

$\rightarrow$ *Alignment phase transition*

$\rightarrow$ *Motility Induced Phase Separation (MIPS)*.

Alignment phase transition

Alignment

Alignment dynamics will create groups of particles moving together and adapting their speed

Original model by Vicsek&al. (1995, *Novel type of phase transition in a system of self driven particles*)

$\mapsto N = \rho L^2$ particles move in the periodic domain $[0, L]^2$, with speed $v_i(t) = v\vec{e}_{\theta_i(t)}$

$$\begin{cases} x_i(t+1) = x_i(t) + v_i(t)\Delta t \\ \theta_i(t+1) = \langle \theta(t) \rangle_r + \xi_\eta \end{cases}$$

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Numerous results and related models

- *Revisiting the flocking transition using active spins*, Solon & Tailleur, 2013
- *Pattern formation in flocking models: A hydrodynamic description*, Solon & al., 2015

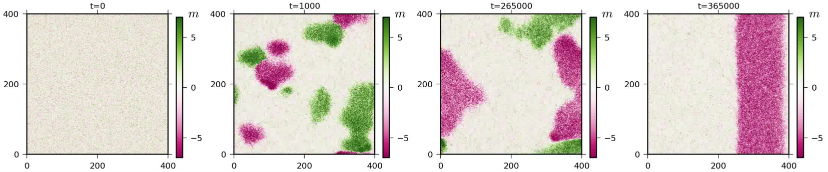


Figure: Emergence of global order for an alignment dynamics. From *Flocking with discrete symmetry, the 2d active Ising model*, Solon & Tailleur 2015.

Exact works

Several analysis and PDE based papers, 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

Particles will tend to accumulate where they move more slowly

- MIPS can occur when the particle's velocity depends on the local density
- MIPS usually does not occur in models with alignment : dense clusters tend to quickly align and spread out

- *When are active Brownian particles and run-and-tumble particles equivalent ? consequence for MIPS*, Cates & Tailleur 2012
- *Motility-induced phase separation*, Cates & Tailleur 2014

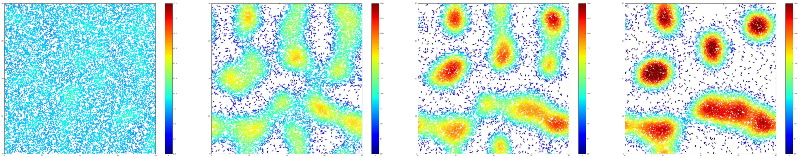


Figure: Coarsening effect in active matter. From Cates & Tailleur 2012.

Plan of the talk

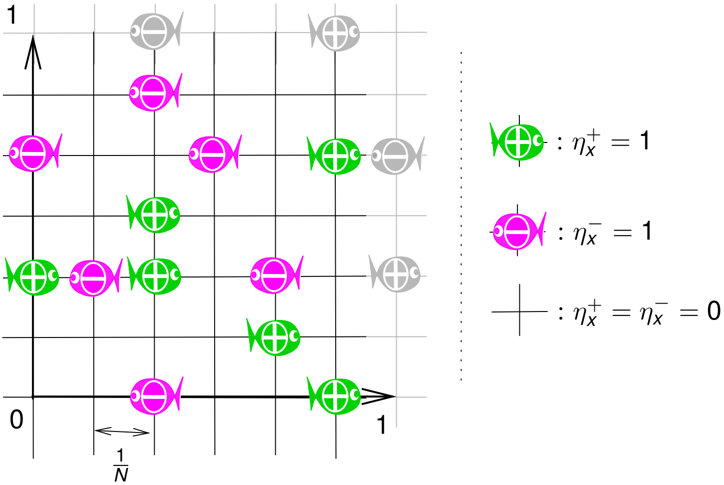
Description of the particle system

$\mapsto$ very close to the Active Ising Model (Solon & Tailleur 2015), with at most one particle per site and weak asymmetry.

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

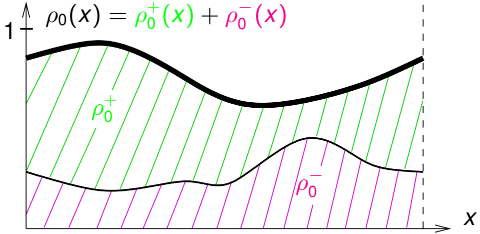
- For each site $x \in \mathbb{T}_N^2$, we define $\eta_x \in \{-1, 0, 1\}$.
  $\mapsto \eta_x = 0$ for an empty site
  $\mapsto \eta_x = \pm 1$ for a site occupied by a particle $\pm$
- We let $\eta_x = \eta_x^+ - \eta_x^-$, where $\eta_x^\pm = 1$ iff x is occupied by a $\pm$ particle.

System configuration



Initial configuration

- Initial setup : **smooth macroscopic 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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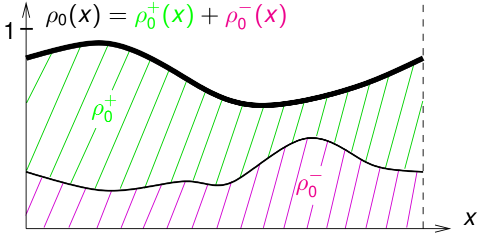

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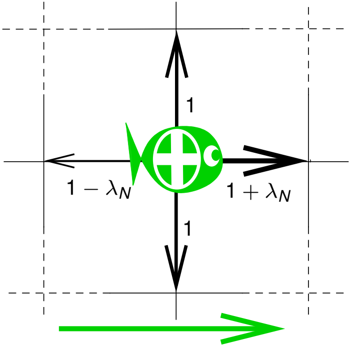
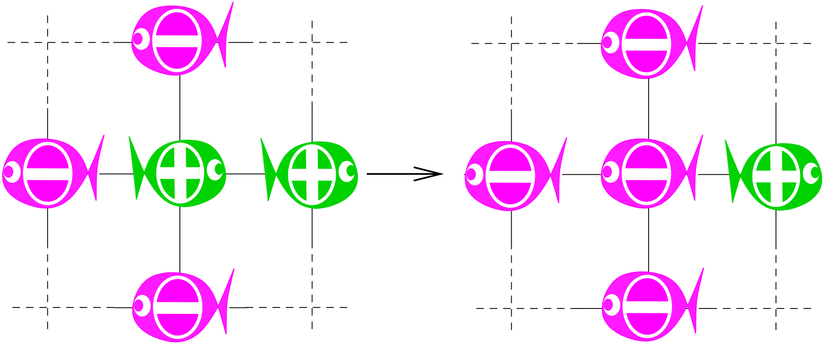
Weakly asymmetric exclusion



- ***Exclusion rule*** : if the target site is occupied, the motion is canceled
- $\lambda_N = \lambda/N$ is the strength of the ***weak asymmetry***

Glauber dynamics



$\mapsto$ *Ising type* alignment dynamics with inverse temperature β

- $\beta = 0$, no alignment
- $\beta \to \infty$, strong alignment

Generator of the dynamic

The Markov generator of the process is given by

$$L_N = N^2 \mathcal{L}^S + \lambda N \mathcal{L}^A + \mathcal{L}^G,$$

- $\mathcal{L}^S$: "generator" of the *Symmetric Simple Exclusion Process* (SSEP)

$$\mathcal{L}^S f(\eta) = \sum_{x \in \mathbb{T}_N} \sum_{|z|=1} |\eta_x| \underbrace{(1 - |\eta_{x+z}|)}_{\text{Exclusion Rule}} \left(f(\eta^{x,x+z}) - f(\eta) \right).$$

- Diffusive scaling : $\times N^2$.

Generator of the dynamic

$$L_N = N^2\mathcal{L}^S + \lambda N\mathcal{L}^A + \mathcal{L}^G,$$

- $\mathcal{L}^A$: generator of the *Asymmetric Simple Exclusion Process* (WASEP)

$$\mathcal{L}^A f(\eta) = \sum_{x\in\mathbb{T}_N}\sum_{\delta=\pm1} \delta\eta_x \underbrace{(1-|\eta_{x+\delta e_1}|)}_{\text{Exclusion Rule}} \Big(f(\eta^{x,x+\delta e_1}) - f(\eta)\Big),$$

- Ballistic scaling : $\times N$.

Generator of the dynamic

$$L_N = N^2\mathcal{L}^S + \lambda N\mathcal{L}^A + \mathcal{L}^G,$$

- $\mathcal{L}^G$: generator of the *Glauber alignment dynamics*

$$\mathcal{L}^G f(\eta) = \sum_{x\in\mathbb{T}_N} c_\beta(x,\eta)|\eta_x|\left(f(\eta^x) - f(\eta)\right).$$

- One can choose for example

$$c_\beta(x,\eta) = \frac{1}{Z_\beta}\exp\left(-\beta\sum_{y\sim x}\eta_x\eta_y\right).$$

- No need for rescaling.

Plan of the talk

Hydrodynamic Limit

Question : Evolution of the macroscopic densities $\rho^+, \rho^- : [0, T] \times [0, 1]^2 \to [0, 1]$?

Weak formulation of the macroscopic evolution

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

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

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Heuristic formulation of the macroscopic limit

Theorem

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 cross reaction-diffusion system*

$$\begin{cases} \partial_t \rho^+ = \nabla.\left[d_s(\rho)\nabla\rho^+ + \mathfrak{d}(\rho^+,\rho)\nabla\rho\right] + 2\lambda\partial_{x_1}\mathfrak{s}^+(\rho^+,\rho) + \Gamma_\beta(\rho^+,\rho) \\ \partial_t \rho^- = \nabla.\left[d_s(\rho)\nabla\rho^+ + \mathfrak{d}(\rho^-,\rho)\nabla\rho\right] + 2\lambda\partial_{x_1}\mathfrak{s}^-(\rho^-,\rho) - \Gamma_\beta(\rho^+,\rho) \end{cases},$$

with initial condition

$$(\rho^+,\rho^-)(0,x) = (\rho_0^+,\rho_0^-)(x) \quad \forall x.$$

The quantity $\rho = \rho^+ + \rho^-$ is the total particle density.

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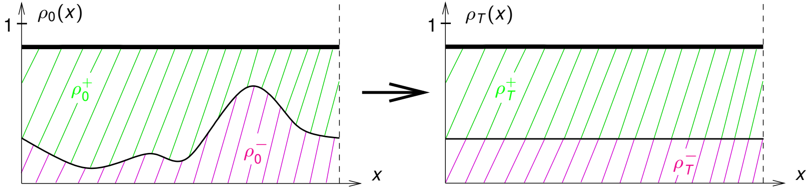
J. Quastel.
Diffusion of colour in the simple exclusion process.
COMM. PURE APPL. MATH, 1992.

S.R.S Varadhan.
Non-linear diffusion limit for a system with nearest neighbor interactions II.
Asymptotic problems in probability theory : Stochastic models and diffusion on fractals, 1994.

C. Kipnis and C. Landim.
Scaling limits of interacting particle systems.
Fundamental Principles of Mathematical Sciences, 1999.

Dynamical interpretation

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



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

Self-diffusion coefficient

Setup :

- infinite SSEP on $\mathbb{Z}^2$ at equilibrium with density $\rho \in]0,1[$.
- At the origin, we place a *tagged particle*.
- $(X_1(t), X_2(t))$ denotes the position at time t of the tagged particle.

Definition

The *self-diffusion coefficient* is defined by

$$d_s(\rho) = \lim_{t\to\infty} \frac{\mathbb{E}(X_1(t)^2)}{t}$$

$\mapsto$ $d_s(\rho)$ can be defined by a variational formula (Spohn, 1990).

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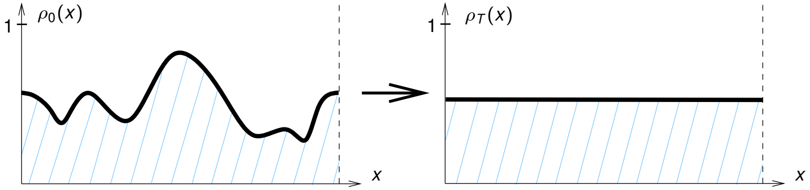

The coefficient $\mathfrak{d}$ quantifies the **diffusion** due to heterogeneities of the **total particle density**

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

Dynamical interpretation

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

$\mapsto$ The drift terms $\mathfrak{s}^+$ and $\mathfrak{s}^-$ can be expressed as

$$\mathfrak{s}^+(\rho^+, \rho) = \rho^+ d_s(\rho) \; + \; \frac{\rho^+}{\rho}(1 - \rho - d_s(\rho))(\rho^+ - \rho^-),$$

$$\mathfrak{s}^-(\rho^-, \rho) = -\rho^- d_s(\rho) \; + \; \frac{\rho^-}{\rho}(1 - \rho - d_s(\rho))(\rho^+ - \rho^-),$$

and are linked to $\mathfrak{d}$ and d_s by a matrix Stokes-Einstein relation.

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- Γ_β is the creation rate of $''+''$ particles.
- It depends on the alignment jump rates c_β

Hydrodynamic limit

Empirical measures

$$\pi_t^{+,N} = \frac{1}{N^2}\sum_{x\in\mathbb{T}_N^2} \eta_x^+(t)\delta_x, \quad \text{and} \quad \pi_t^{-,N} = \frac{1}{N^2}\sum_{x\in\mathbb{T}_N} \eta_x^-(t)\delta_x.$$

We want to prove $\pi_t^{+,N} \to \pi_t^+ = \rho^+(t,x)dx$, i.e. that for any smooth H,

$$< \pi_t^{+,N}, H > \to \int_{[0,1]^2} \rho^+(t,x)H(x)dx$$

Core principle :

$$< \pi_T^{+,N}, H > = < \pi_0^{+,N}, H > + \int_0^T L_N < \pi_t^{+,N}, H > dt + \overbrace{M_T^N}^{o_N(1)}$$

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Hydrodynamic limit

Assume we are in **one dimension** :

$$
\begin{aligned}
L_N < \pi_t^{+,N}, H > &= \frac{1}{N} \sum_{x \in \mathbb{T}_N} H(x) L_N \eta_x^+ \\
&= \frac{1}{N} \sum_{x \in \mathbb{T}_N} H(x) \left(W_{x-\frac{1}{N},x} - W_{x,x+\frac{1}{N}} + \gamma_{\beta,x} \right) \\
&= \frac{1}{N} \sum_{x \in \mathbb{T}_N} \left[\left(H(x) - H\left(x + \frac{1}{N}\right)\right) W_{x,x+\frac{1}{N}} + H(x)\gamma_{\beta,x} \right]
\end{aligned}
$$

and the instantaneous particle current can be written

$$
W_{x,x+\frac{1}{N}} = N^2 \underbrace{w^S_{x,x+\frac{1}{N}}}_{\text{symmetric current}} + \lambda N \underbrace{w^A_{x,x+\frac{1}{N}}}_{\text{antisymmetric current}} .
$$

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Non-gradient hydrodynamics

- The partial derivative on H balances out a factor N in the current.
- In ***non-gradient systems***, the symmetric current $w^S_{x,x+\frac{1}{N}}$ is not a discrete gradient.
  $\mapsto$ the second integration by parts is not immediate
- One must prove

$$N.w^S_{x,x+\frac{1}{N}} \simeq N\left[d_s(\eta^+_x - \eta^+_{x+1}) + \mathfrak{d}(|\eta_x| - |\eta_{x+1}|) + \mathcal{L}^S f\right]$$

Key steps in the hydrodynamic limit

Additionally to the justification of this replacement, some key points are needed :

- Prove that the measure of the process is ”close” to a product measure : *conservation of local equilibrium*
- Introduce *spatial averages*
- Prove a *law of large number for the process*, and replace, for example, the spatial average of $\eta_x^+(t)$ by the density $\rho^+(t,x)$

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Out of equilibrium dynamics

Key issue

Comparison with a product measure on the discrete lattice :

- Distortion of the measure by the Glauber part and the initial configuration are easily controlled
- Distortion by the weak drift, harder to control

$\mapsto$ Challenge : prove that the exponential estimates needed in the *non-gradient* method still hold.

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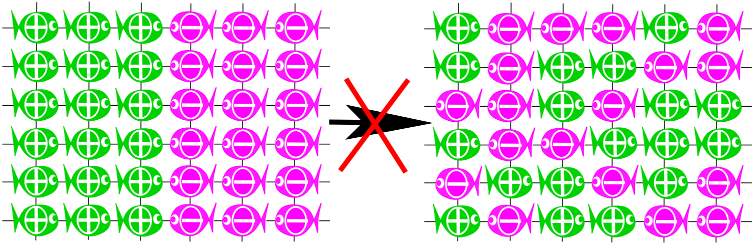
Irreducibility

Exclusion rule : the process is not always irreducible on canonical ensembles with fixed number and types of particles.



Irreducibility

- One must prove that the dynamics preserves sufficient empty sites spread in the configuration to ensure mixing.
- This was a major issue with the model, which was not present in Quastel's symmetric case.
- Let

$$F_p(x) = \{\text{There is no empty site in } B_p(x)\},$$

one must in particular prove that

$$\mathbb{E}\left(\frac{1}{N^2}\sum_{x\in\mathbb{T}_N} \mathbb{1}_{F_p(x)}\right) \underset{N\to\infty}{\simeq} \int_{[0,1]^2} dx\, \rho_x^{|B_p|} \underset{p\to\infty}{\longrightarrow} 0. \qquad (1)$$

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one must in particular prove that

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Irreducibility

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Elements on the proof of (1)

The total density $\rho = \rho^+ + \rho^-$ is expected to satisfy

$$\partial_t \rho = \Delta \rho + \lambda \partial_{x_1}(m(1-\rho)), \qquad (2)$$

where $m = (\rho^+ - \rho^-)$ denotes the local "magnetization" of the system.

- Analysis-based proof with microscopic methods, using (2)
- The proof relies on the a-priori control of the density and Gronwall's Lemma

Elements on the proof of (1)

Let $\phi(\rho) = 1/(1-\rho)$, one can prove, assuming (2), that

$$\partial_t \int_{\mathbb{T}} \phi(\rho_t)dx \leq 2\lambda^2 \int_{\mathbb{T}} \phi(\rho_t)dx$$

$\mapsto$ By Gronwall's Lemma, at any time t,

$$\int_{\mathbb{T}} \phi(\rho_t)dx \leq e^{Ct} \underbrace{\int_{\mathbb{T}} \phi(\rho_0)dx}_{<\infty \text{ by assumption}}.$$

The right-hand side remains finite, therefore the total density cannot reach 1.

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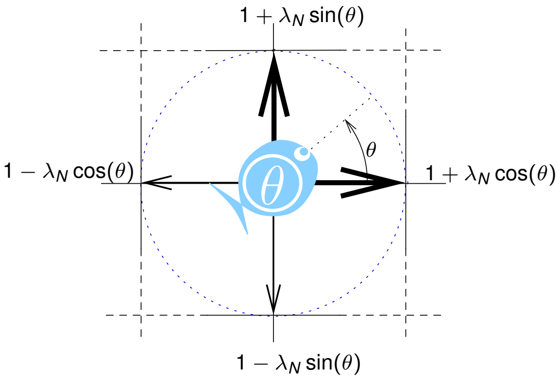
Plan of the talk

Continuous angles dynamic

- The two particle types $+$ and $-$ can be interpreted as angles 0 and π for the drift.
- We now want to extend the proof of the hydrodynamic limit to an angle continuum $\theta \in [0, 2\pi[$.



Main result

The macroscopic density ρ^θ of particles with angle θ, can be "défined" as

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

Theorem (Continuous angles)

Assumption : $\forall x \in [0,1]^2,\ \rho_0(x) < 1.$

The "function" $(t,x,\theta)\mapsto\rho^\theta(t,x)$ *is solution* ***in a weak sense*** *of*

$$\partial_t\rho^\theta = \nabla.\left[d_s(\rho)\nabla\rho^\theta + \mathfrak{d}(\rho^\theta,\rho)\nabla\rho\right] + \lambda\nabla.\overrightarrow{\mathfrak{s}}(\rho^\theta,\overrightarrow{m},\rho) + \Gamma_\beta^\theta,$$

where $\rho = \int_\theta \rho^\theta d\theta$ *is the total particle density.*

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Proof in the continuous case

- Local equilibrium is no longer characterized by a finite number of parameters (e.g. ρ^+ and ρ^-)
- Instead, local equilibrium is characterized by an angle measure on $[0, 2\pi[$: if, locally, one observes $1/3$ of empty sites, $1/3$ of particles with angle 0 and $1/3$ with angle π, the corresponding measure is

$$\widehat{\alpha} = \frac{1}{3}\delta_0 + \frac{1}{3}\delta_\pi$$

- This creates several technical difficulties, but the principle of the proof still holds.

Research perspectives

- Replacing metric interactions by topological interactions, typically with the k-nearest neighbors : this should be possible with similar density control tools.
- Large deviations for the system (Macroscopic fluctuations theory)
- Dynamical phase transition (Much harder)

Thanks for your attention !