Statistical mechanics for the phase separation of interacting self propelled particles

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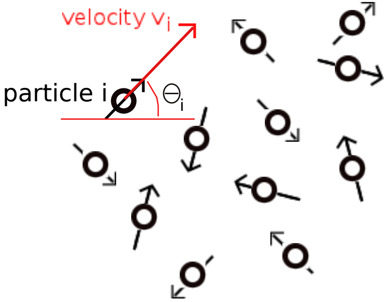
Discovering the joys of research with Stefano

1998 World Cup, Italy vs France. L. Di Biagio misses his penalty kick.

Self propelled particles

- Particles with an internal source of free energy that they can convert into systematic movement.
- Used to model flocks of animals (from mammals to insects), bacteria, some artificial systems... This will be a theoretical talk!
- Main question: understand their collective properties
- Blooming field; many recent developments (I will not be able to cite all relevant contributions!).

The model system (2D)



- Point particles with an internal angular variable θ_i
- Move with speed v_i along direction θ_i + spatial noise
- the speed v_i may depend on the local density
- Particles interact: they tend to align locally

Microscopic equations (2D)

• Spatial variables: transport in direction θ_i (speed may depend on local density) + noise
• Angular variables: interactions promoting local alignment + noise

$$
\begin{aligned}
\dot{\mathbf{x}}_i &= v(n_i)\mathbf{u}(\theta_i) + \sqrt{2D_x}\sigma_i(t) \\
\dot{\theta}_i &= -\frac{\gamma}{n_i} \sum_{j \text{ neighbor of } i} \sin(\theta_i - \theta_j) + \sqrt{2D_\theta}\eta_i(t)
\end{aligned}
$$

with

$$
\begin{aligned}
n_i &= \text{local density} \\
\sigma_i,\ \eta_i &= \text{gaussian white noises, unit covariance}
\end{aligned}
$$

Representative of a class of models with similar large scale properties.

Qualitative behavior

• Strong interactions, or "external field" $\rightarrow$ local orientation order. Not studied here.

• Weak interactions $\rightarrow$ no local orientation order
Large scale dynamics = diffusive.

• v depends on the local density $\rho \rightarrow$ effective diffusion coefficient depends on ρ
Possibility of "motility induced phase separation" (Cates, Tailleur)

Main questions

- A macroscopic description? Finite N fluctuations? Stationary measure? Probability distribution of the density?
- A very quick review
  - J. Toner, Y. Tu (1995): phenomenological hydrodynamical equations + noise introduced "by hand"
  - E. Bertin, M. Droz, G. Grégoire (2006): write a Boltzmann like equation + expansion close to the phase transition threshold $\rightarrow$ derivation of Toner-Tu like equations, without noise (many developments from there: Chaté et al., Marchetti et al., Ihle...)
  - Math. literature: P. Degond, S. Motsch (2007); Fokker-Planck like models (locally mean-field); far from the threshold
  - Keeping finite N fluctuations: J. Tailleur, M. Cates et al. (2008, 2011, 2013): without alignment promoting interactions; Bertin et al. (2013): derive a noise from the microscopic equations for nematics.

Our goals

1. start from microscopic equations
2. derive hydrodynamical equations and noise in a controlled way Noise may have correlations $\rightarrow$ important to have a microscopic derivation
3. exploit these results to study the dynamical fluctuations of the empirical density (cf Macroscopic Fluctuation Theory).
4. obtain large deviation estimate for the stationary spatial density ρ such as
$$\mathbb{P}(\rho \approx u) \asymp e^{NS[u]}$$
$S =$ "entropy", or "quasi-potential".

Simple framework: aligning interactions below threshold for local order; density dependent speed ($\rightarrow$ clustering possible).

Microscopic equations (simplified), adimensionalized

$$\frac{d\tilde{\mathbf{x}}_i}{d\tilde{t}} = \varepsilon \tilde{v}(n_i)\mathbf{u}(\theta_i) + \varepsilon\sqrt{2\tilde{D}_x}\vec{\sigma}_i(\tilde{t}) \quad (1)$$

$$\frac{d\theta_i}{d\tilde{t}} = -\frac{\tilde{\gamma}}{n_i} \sum_{j \text{ neighbor of } i} \sin(\theta_i - \theta_j) + \sqrt{2}\,\eta_i(\tilde{t})\,, \quad (2)$$

with $\varepsilon = v_0/(LD_\theta)$, $\tilde{D}_x = D_x D_\theta / v_0^2$, $\tilde{\gamma} = \gamma/D_\theta$, $\tilde{t} = D_\theta t$.

Two important parameters:
$\tilde{D}_x$: ratio spatial diffusion/"active" diffusion
$\tilde{\gamma}$: strength of the aligning interaction

$\varepsilon =$ spatial time scale/angular time scale: small parameter

Strategy

Main object of interest: the empirical density

$$\rho(\mathbf{x}, \theta, t) = \frac{1}{N} \sum_i \delta(\mathbf{x} - \mathbf{x}_i(t))$$

Phase space empirical density

$$f(\mathbf{x}, \theta, t) = \frac{1}{N} \sum_i \delta(\mathbf{x} - \mathbf{x}_i(t)) \delta(\theta - \theta_i(t))$$

1. Write an equation for f that keeps finite N fluctuations (cf D. Dean 1996): in a sense exact in the large N limit
2. Use the time-scale separation to write an equation for ρ that keeps finite N fluctuations: hoped to be exact in a combined $\varepsilon \to 0$, $N \to \infty$ limit
3. Write a functional Fokker-Planck equation for $\mu_t[\rho]$, the pdf of ρ.
4. Look for a stationary solution of the form

$$\mu[\rho] \asymp e^{NS[\rho]}$$

A fluctuating non linear Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \overbrace{-\varepsilon \nabla \left(v(\rho)\mathbf{u}(\theta) f \right)}^{\text{transport}} + \overbrace{\frac{\gamma}{\rho}\frac{\partial}{\partial \theta}\left(f \int d\theta' \sin(\theta - \theta') f(\theta') \right)}^{\text{interaction}}$$

$$\underbrace{+ \sqrt{\frac{2}{N}}\frac{\partial}{\partial \theta}\left(\eta(\mathbf{x}, \theta, t)\sqrt{f} \right) + \varepsilon \frac{\sqrt{2D_x}}{\sqrt{N}} \nabla_x \cdot \left(\vec{\sigma}(\mathbf{x}, \theta, t)\sqrt{f} \right)}_{\text{finite N fluctuations}}$$

$$+ \quad \underbrace{\frac{\partial^2 f}{\partial \theta^2} + \varepsilon^2 D_x \nabla_x^2 f}_{\text{angular and spatial diffusions}}$$

Meaning? A dynamical large deviation principle (Dawson 1987).

$$\mathbb{P}(f_t \approx g_t) \asymp \exp(-N J_{[0,T]}[g]) \; ; \; J_{[0,T]}[g] = \frac{1}{4}\int_0^T ||\partial_t g - VFP[g]||^2_{-1,g} dt$$

VFP = nonlinear Vlasov-Fokker-Planck operator= red terms

On the computations

• Local equilibrium + small deviation (order ε and $1/\sqrt{N}$ fluctuations)

$$f(\mathbf{x},\theta,t) = \frac{1}{2\pi}\rho(\mathbf{x},\varepsilon^{\alpha}t) + \delta f(\mathbf{x},\theta,t)$$

• Equation for ρ: slow time scale, depends on δf

$$\frac{\partial\rho}{\partial t} = -\varepsilon\nabla(v\int u_{\theta}\delta f) + \varepsilon^2 D_x\nabla^2\rho + \varepsilon\frac{\sqrt{2D_x}}{\sqrt{N}}\nabla\cdot\left(\vec{\xi}(x,y,t)\right) \quad (3)$$

$\xi =$ noise, multiplicative in ρ.

• δf small $\rightarrow$ obtained by solving a linearized equation

• Reintroduce into Eq.(3) $\rightarrow$ the final equation, a fluctuating PDE for ρ.

Dynamical large deviation principle

- Fluctuating PDE for ρ

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= U[\rho](\vec{x}) + \frac{1}{\sqrt{N}}\nu(\vec{x},t) \\ U[\rho](\vec{x}) &= \frac{1}{2}\nabla\cdot\left(\frac{v(\rho)}{1-\frac{\bar{\gamma}}{2}}\nabla[v(\rho)\rho]\right) + D_x\nabla^2\rho \\ \langle \nu(x,y,t)\nu(x',y',t')\rangle &= D[\rho](\vec{x},\vec{x}')\delta(t-t') \end{aligned}$$

- The fluctuating PDE for ρ is a rephrasing of a dynamical large deviation principle "à la Dawson"

$$\mathbb{P}(\rho \approx u) \asymp \exp(-NI_{[0,T]}[u]) \text{ with } I_{[0,T]}[u] = \frac{1}{2}\int_0^T ||\partial_t u - U[u]||^2_{-1,D}$$

- This kind of dynamical large deviation principle is the starting point for the macroscopic fluctuation theory (in this case, it is actually trivial...)

Yet another formulation: functional Fokker-Planck equation

• Ordinary stochastic differential equation for $x \in \mathbb{R}^d \to$ PDE (Fokker-Planck) for the pdf of x.
• Stochastic PDE for a field $\rho \to$ functional equation for $\mu_t[\rho]$, "pdf" of ρ.

$$\frac{\partial \mu_t}{\partial t} = \overbrace{-\int d\vec{x} \frac{\delta}{\delta \rho(\vec{x})} \left(U[\rho](\vec{x}) \mu_t \right)}^{\text{drift part}} \\ + \underbrace{\frac{1}{2N} \int d\vec{x} \frac{\delta}{\delta \rho(\vec{x})} \left\{ \int d\vec{x}' D[\rho](\vec{x}, \vec{x}') \frac{\delta}{\delta \rho(\vec{x}')} \mu_t \right\}}_{\text{diffusion part}}$$

Results and discussion

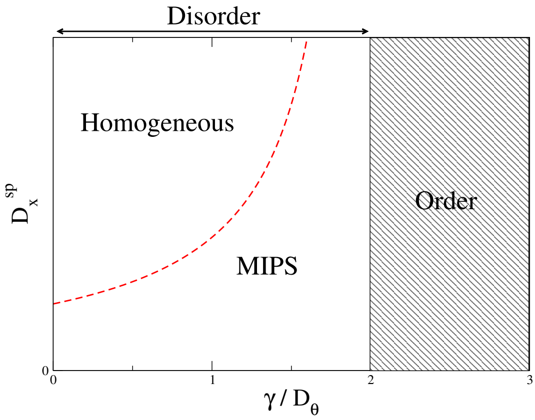
• When $\gamma < \gamma_c$, system effectively at equilibrium (case without aligning interactions: Cates, Tailleur et al. 2007, 2011, 2013)
$\rightarrow$ computing S is possible, $S[\rho] = \int s(\rho(\mathbf{x}))d\mathbf{x}$

$$s''(\rho) = -\left(\frac{v^2(\rho) + \rho v(\rho)v'(\rho)}{\left(1 - \frac{\bar{\gamma}}{2}\right) b[\rho]} + \frac{2D_x}{b[\rho]}\right)$$

• $\rightarrow$ compute $S[\rho]$

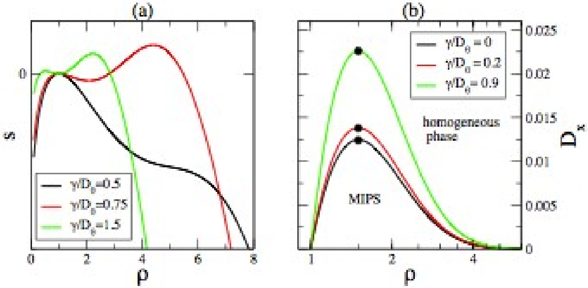
Results and discussion

- Reasonable to assume $v(\rho)$ decreasing $\rightarrow$ possible phase separation (MIPS = Motility Induced Phase Separation). Role of the interactions?



Sketch of the $D_x - \tilde{\gamma}$ phase diagram.

Results and discussion



Left: entropy $s(\rho)$. Right: $D_x - \rho$ phase diagram.

- Spinodal line very sensitive to the interaction strength (observed in simulations)
- Density fluctuations increase when approaching the ordered phase
- A strong enough spatial diffusion always prevent phase separation

Conclusion

- Nice example where the limiting procedures seem well controlled + a general strategy
- Some physical insight in the "Motility Induced Phase Separation" with aligning interactions
- Next step: with a local orientation order
  $\rightarrow$ hyperbolic hydrodynamic limit
  $\rightarrow$ one cannot expect an effective equilibrium in the same sense
- Mathematical theory much less developed in this case... (recent works by Mariani, Bertini et al.) Work in progress...