Kinetic theory and hydrodynamic equations for systems of self-propelled particles

Eric Bertin

LIPhy, Univ. Joseph Fourier, Grenoble

Collab.: H. Chaté, G. Grégoire, S. Léonard, S. Ngo, A. Peshkov (Paris), F. Ginelli (Aberdeen), M. Droz (Geneva), I.S. Aronson (Argonne), S. Ramaswamy (Hyderabad)

Workshop "Collective Motion of Active Swimmers", Nice, September 25-26, 2013

Motivation: a physicist viewpoint

- Self-propelled agents are common in nature (birds flocks, fish schools, bacteria colonies), and in manufactured "objects" (robots, cars...)
- In some instances, a spontaneous collective motion emerges (no leader, no external cause)

Motivation: a physicist viewpoint

- How to describe this transition to motion?
- Can one propose a coarse-grained description with hydrodynamic equations?
- Is it possible to derive hydrodynamic equations from a microscopic model?

Vicsek model

- Point-like particles with fixed velocity modulus, and noisy alignment interactions with neighboring particles
- Direct simulations in 2D:
  transition to motion observed when reducing the noise

  T. Vicsek et. al., PRL **75**, 1226 (1995)

Large-scale simulations

- Transition toward motion confirmed
- At very large sizes ($\sim 10^5 - 10^6$ particles):
  onset of spatially inhomogeneous states

  G. Grégoire, H. Chaté, PRL **92**, 025702 (2004)

Analytical approaches

Hydrodynamic equations based on symmetry considerations

- Phenomenological generalized Navier-Stokes equation including all terms allowed by the symmetries
- Less symmetries than in usual fluids, due in particular to the absence of galilean invariance
- Drawback: the coefficients entering the hydrodynamic equation have no microscopic content

Renormalization approaches

Dynamic renormalization group

$\Rightarrow$ long-range order is stable in dimension $d = 2$

J. Toner and Y. Tu, PRL **75**, 4326 (1995)

In this talk

Systems considered

- Different microscopic models of DRY active matter (particles on a substrate, with no surrounding fluid)
- Common feature: motion along particle's orientation (either directed motion or random vibration)
- Different interaction symmetries: "ferromagnetic" or nematic

Main results

- Derivation of continuous equations for polar and/or nematic order parameters
- Study of their behavior: instabilities, onset of order, non-linear patterns

OUTLINE

- *Polar self-propelled particles with "ferromagnetic" velocity alignment*
- *Polar self-propelled particles with nematic velocity alignment*
- *Active nematic particles*

OUTLINE

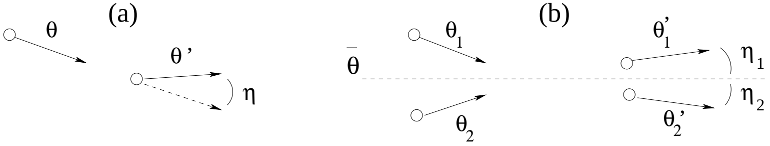
- *Polar self-propelled particles with "ferromagnetic" velocity alignment*
- *Polar self-propelled particles with nematic velocity alignment*
- *Active nematic particles*

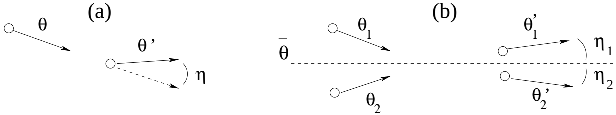
Self-propelled particles

- Point-like particles, in a 2D plane, with velocity $\mathbf{v}$ of fixed magnitude v_0
- Velocity simply defined by the angle θ

Stochastic dynamics

- Self-diffusion of isolated particles
- Binary collisions when the distance between two particles becomes less than an interaction radius d_0





(a) Self-diffusion

- New angle $\theta' = \theta + \eta \, [2\pi]$
- η a Gaussian noise with variance σ_0^2, distribution $p_0(\eta)$

(b) Binary collisions

- Define the average angle $\overline{\theta} = \mathrm{Arg}(e^{i\theta_1} + e^{i\theta_2})$
- New angles $\theta'_1 = \overline{\theta} + \eta_1$ and $\theta'_2 = \overline{\theta} + \eta_2$
- η a Gaussian noise with variance σ^2 that may differ from σ_0^2, and distribution $p(\eta)$

Self-propelled particles with velocity alignment

Principle of the description

- Evolution equation for the one-particle phase-space distribution $f(\mathbf{r}, \theta, t) =$ probability to find a particle at time t in $\mathbf{r}$, with a velocity angle θ
- Approximation scheme: factorize the two-particle distribution as a product of one-particle distributions (low density)

Boltzmann equation

$$\frac{\partial f}{\partial t}(\mathbf{r}, \theta, t) + v_0\, \mathbf{e}(\theta) \cdot \nabla f(\mathbf{r}, \theta, t) = I_{\mathrm{dif}}[f] + I_{\mathrm{col}}[f]$$

Bertin, Droz, Grégoire, Phys. Rev. E 2006 and J. Phys. A 2009

See also Carlen, Chatelin, Degond, Wennberg, Physica D (2013).

Integral terms in the Boltzmann equation

Self-diffusion term

$$I_{\mathrm{dif}}[f] = -\lambda f(\mathbf{r},\theta,t) + \lambda \int_{-\pi}^{\pi} d\theta' \int_{-\infty}^{\infty} d\eta \, p_0(\eta) \delta_{2\pi}(\theta' + \eta - \theta) \, f(\mathbf{r},\theta',t)$$

Binary collision term

[with $\overline{\theta} = \mathrm{Arg}(e^{i\theta_1} + e^{i\theta_2})$]

$$I_{\mathrm{col}}[f] = -f(\mathbf{r},\theta,t) \int_{-\pi}^{\pi} d\theta' \, |\mathbf{e}(\theta') - \mathbf{e}(\theta)| f(\mathbf{r},\theta',t) + \int_{-\pi}^{\pi} d\theta_1 \int_{-\pi}^{\pi} d\theta_2 \int_{-\infty}^{\infty} d\eta \, p(\eta) \, |\mathbf{e}(\theta_2) - \mathbf{e}(\theta_1)| \, f(\mathbf{r},\theta_1,t) \, f(\mathbf{r},\theta_2,t) \times \delta_{2\pi}(\overline{\theta} + \eta - \theta)$$

Self-propelled particles with velocity alignment

Hydrodynamic fields

- Density field

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

- Velocity field $\mathbf{u}(\mathbf{r},t)$ and momentum field $\mathbf{w}(\mathbf{r},t)$

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

Continuity equation

Integration of Boltzmann equation over θ

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

Velocity-field equation ("Navier-Stokes")

- Principle: multiply Boltzmann equation by $\mathbf{v} = v_0\,\mathbf{e}(\theta)$ and integrate over θ
- Not a closed equation in terms of ρ and $\mathbf{u}$: need for an approximation scheme
- Fourier series expansion over the angle θ: $f(\mathbf{r},\theta,t) \to \hat{f}_k(\mathbf{r},t)$
- Truncation and closure scheme, valid for small $|\mathbf{w}| = \rho|\mathbf{u}|$ (scaling ansatz close to instability threshold)

$$\frac{\partial \mathbf{w}}{\partial t} + \gamma(\mathbf{w}\cdot\nabla)\mathbf{w} = -\frac{1}{2}\nabla(\rho - \kappa \mathbf{w}^2) + \left(\mu(\rho) - \xi \mathbf{w}^2\right)\mathbf{w} + \nu\nabla^2\mathbf{w} - \kappa(\nabla\cdot\mathbf{w})\mathbf{w}$$

E. Bertin, M. Droz, G. Grégoire, PRE **74**, 022101 (2006) & J. Phys. A **42**, 445001 (2009)

Transport coefficients

$$\nu = \frac{1}{4}\left[\lambda\left(1 - e^{-2\sigma_0^2}\right) + \frac{4}{\pi}\rho\left(\frac{14}{15} + \frac{2}{3}e^{-2\sigma^2}\right)\right]^{-1}$$

$$\gamma = \frac{8\nu}{\pi}\left(\frac{16}{15} + 2e^{-2\sigma^2} - e^{-\sigma^2/2}\right)$$

$$\kappa = \frac{8\nu}{\pi}\left(\frac{4}{15} + 2e^{-2\sigma^2} + e^{-\sigma^2/2}\right)$$

$$\mu = \frac{4}{\pi}\rho\left(e^{-\sigma^2/2} - \frac{2}{3}\right) - \lambda\left(1 - e^{-\sigma_0^2/2}\right)$$

$$\xi = \frac{64\nu}{\pi^2}\left(e^{-\sigma^2/2} - \frac{2}{5}\right)\left(\frac{1}{3} + e^{-2\sigma^2}\right)$$

Main result: explicit expression of the transport coefficients as a function of microscopic parameters

Stability of the zero-velocity solution

- Evolution equation for the homogeneous solution $\mathbf{w}(\mathbf{r},t) = \mathbf{w}(t)$

$$\frac{\partial \mathbf{w}}{\partial t} = (\mu - \xi \mathbf{w}^2)\mathbf{w}$$

- Stability of $\mathbf{w} = 0$ related to the sign of μ ($\mu > 0$: unstable)

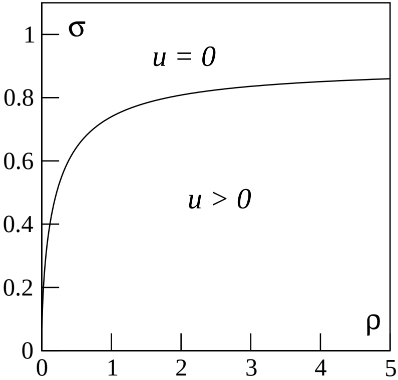
$$\mu = \frac{4}{\pi}\rho\left(e^{-\sigma^2/2} - \frac{2}{3}\right) - \lambda\left(1 - e^{-\sigma_0^2/2}\right)$$

- $\mathbf{w} = 0$ unstable for $\rho > \rho_t$

$$\rho_t = \frac{\pi\lambda(1 - e^{-\sigma_0^2/2})}{4(e^{-\sigma^2/2} - \frac{2}{3})}$$

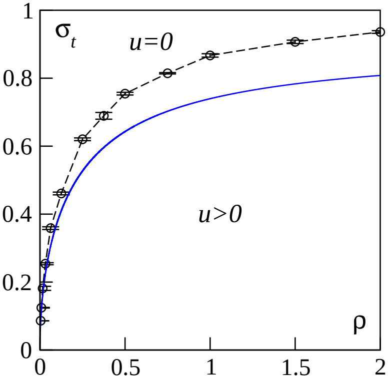
- For $\rho > \rho_t$, homogeneous motion $|\mathbf{w}_0| = \sqrt{\mu/\xi}$, in an arbitrary direction

Phase diagram in the noise-density plane



Phase diagram cannot be predicted from phenomenological equations (noise is a microscopic parameter)

Phase diagram: comparison with the Vicsek model



Qualitative agreement between numerical phase diagram of Vicsek model and analytic phase diagram of binary collision model

$\Rightarrow$ genericity of the hydrodynamic description

Finite wavelength perturbation

- Small perturbation around the homogeneous motion

$$\rho(\mathbf{r},t) = \rho_0 + \delta\rho(\mathbf{r},t), \quad \mathbf{w}(\mathbf{r},t) = \mathbf{w}_0 + \delta\mathbf{w}(\mathbf{r},t)$$

- Finite wavevector $\mathbf{q}$

$$\delta\rho(\mathbf{r},t) = \delta\rho_0\, e^{st+i\mathbf{q}\cdot\mathbf{r}}, \quad \delta\mathbf{w}(\mathbf{r},t) = \delta\mathbf{w}_0\, e^{st+i\mathbf{q}\cdot\mathbf{r}}$$

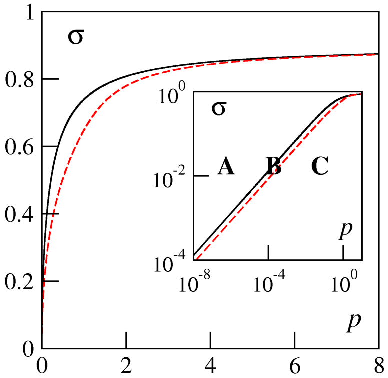
Dispersion relation for $s(\mathbf{q})$

- For small $|\mathbf{q}|$, one finds

$$\Re(s) = \frac{\mu_0^2}{8\,\xi^3 w_0^4}\,|\mathbf{q}|^2 - \frac{5\,\mu_0^4}{128\,\xi^7 w_0^{10}}\,|\mathbf{q}|^4 + \mathcal{O}(|\mathbf{q}|^6)$$

- $\Re(s) > 0$ for small enough $|\mathbf{q}|$ $\Rightarrow$ instability of homogeneous motion against long-wavelength perturbations

Stability diagram



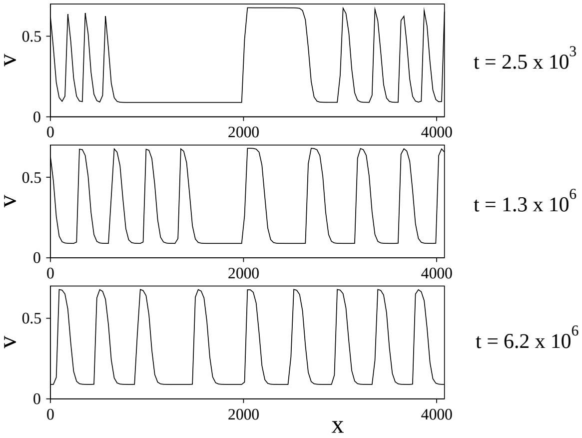
A = no collective motion

B = inhomogeneous flow

C = homogeneous flow

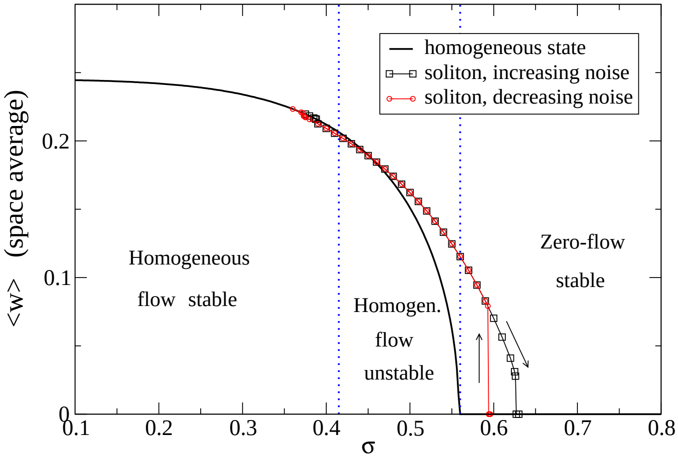
E. Bertin, M. Droz, G. Grégoire, J. Phys. A **42**, 445001 (2009)

Trains of solitary waves in the hydrodynamic equation



A. Peshkov, S. Léonard, E. Bertin, H. Chaté, G. Grégoire, to be published

Varying the noise: hysteresis effect

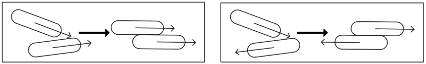


Solitary waves exist even in some regions where the homogeneous state is stable (with or without flow)

- *Polar self-propelled particles with "ferromagnetic" velocity alignment*
- *Polar self-propelled particles with nematic velocity alignment (rods)*
- *Active nematic particles*

Nematic alignment rules

(Ginelli, Peruani, Bär, Chaté, PRL 2010)



Hydrodynamic equations

$f_k(\mathbf{r}, t)$ angular Fourier coefficients

f_1 = polar order parameter; f_2 = nematic order parameter

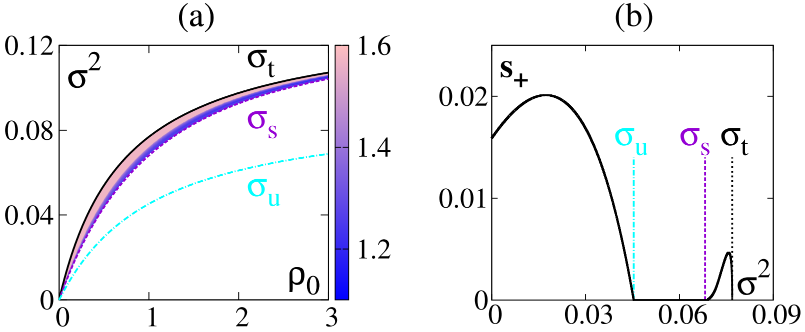
$$\partial_t f_1 = -\frac{1}{2}(\nabla\rho + \nabla^* f_2) + \frac{\gamma}{2} f_2^* \nabla f_2 - (\alpha - \beta|f_2|^2) f_1 + \zeta f_1^* f_2$$

$$\partial_t f_2 = -\frac{1}{2}\nabla f_1 + \frac{\nu}{4}\nabla\nabla^* f_2 - \frac{\kappa}{2} f_1^* \nabla f_2 - \frac{\chi}{2}\nabla^*(f_1 f_2) + \left(\mu(\rho) - \xi|f_2|^2\right) f_2 + \omega f_1^2 + \tau|f_1|^2 f_2$$

$$\nabla \equiv \partial_x + \mathrm{i}\partial_y, \qquad \nabla^* \equiv \partial_x - \mathrm{i}\partial_y$$

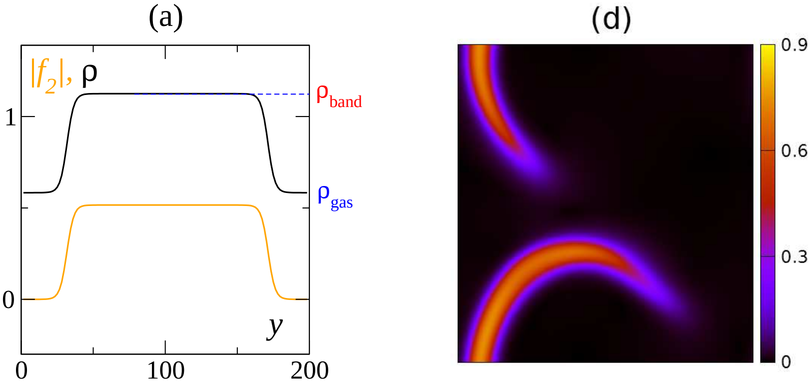
A. Peshkov, I.S. Aronson, E. Bertin, H. Chaté, F. Ginelli, PRL **109**, 268701 (2012)

Stability diagram



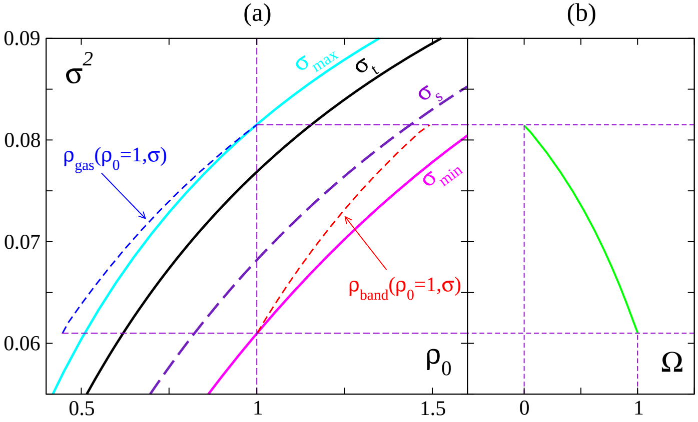
A. Peshkov *et.al.*, PRL (2012)

Band solutions: profile and chaotic regime for f_2



A. Peshkov *et.al.*, PRL (2012)

Existence domain of bands



A. Peshkov *et.al.*, PRL (2012)

OUTLINE

- *Polar self-propelled particles with "ferromagnetic" velocity alignment*
- *Polar self-propelled particles with nematic velocity alignment (rods)*
- *Active nematic particles*

Dynamics of individual particles

- No directed motion (no self-propulsion)
- Random vibration along particle's direction
- Nematic alignment rules

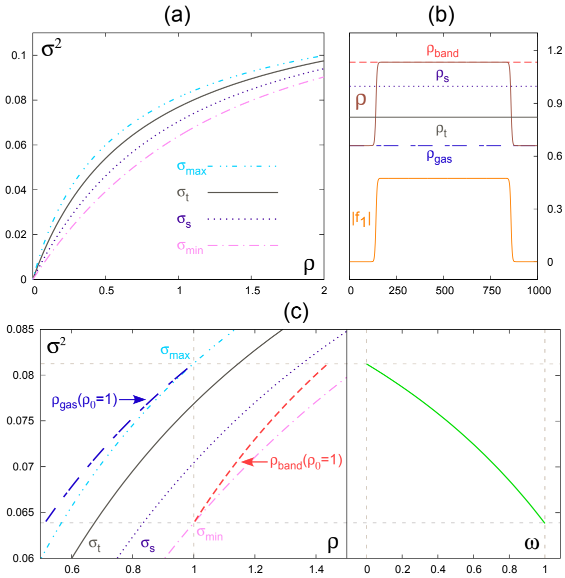
Hydrodynamic equations (f_2 = nematic order parameter)

$$\begin{aligned} \partial_t \rho &= \frac{1}{2}\Delta\rho + \frac{1}{2}\mathrm{Re}\left(\nabla^{*2} f_2\right) \\ \partial_t f_2 &= \left(\mu(\rho) - \xi\,|f_2|^2\right) f_2 + \frac{1}{4}\nabla^2\rho + \frac{1}{2}\Delta f_2 \end{aligned}$$

$$\nabla \equiv \partial_x + \mathrm{i}\partial_y, \qquad \nabla^* \equiv \partial_x - \mathrm{i}\partial_y$$

E. Bertin, H. Chaté, F. Ginelli, S. Mishra, A. Peshkov, S. Ramaswamy, New J. Phys. (2013)

Active nematics: stability diagram



On the methodology

- Generic method to derive continuous equations for **dry** active matter in the low density regime
- Known transport coefficients as a function of microscopic parameters
- Simple phase diagram with only two parameters: density and amplitude of microscopic noise

Conclusion

Genericity of the results

- Onset of order (either polar or nematic depending on interaction symmetries) when crossing a transition line in the noise-density plane
- Generic instability of the homogeneous ordered state close to the transition line
- Formation of ordered bands, that can either be stable or enter a chaotic regime

It would be of high interest to observe such ordered structures experimentally

A potential candidate: experiment on microtubules (see Sumino et.al., Nature 2012)