Collective motion in large deviations of active particles

Y.-E. Keta[1,2,3], É. Fodor[2,4], F. van Wijland[3], M. E. Cates[2], and R. L. Jack[2,5]

[1]Laboratoire Charles Coulomb, UMR 5221 CNRS, Université de Montpellier, France [2]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, United Kingdom [3]Université Paris Diderot, Laboratoire Matière et Systèmes Complexes, UMR 7057 CNRS, F-75205 Paris, France [4]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg [5]Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom

yann-edwin.keta@umontpellier.fr

Motivation

- Large deviations of physical systems consider **transient rare events**, often accompanied by collective effects. Numerical techniques used to analyse these events enable us to study the **microscopic mechanisms which stabilise these atypical collective behaviours**.
- Some large deviations of isotropic active Brownian particles (ABPs) were shown to be associated with **collective motion** (CM), despite the **absence of any microscopic aligning interactions**. We study in greater details this transition to collective motion.

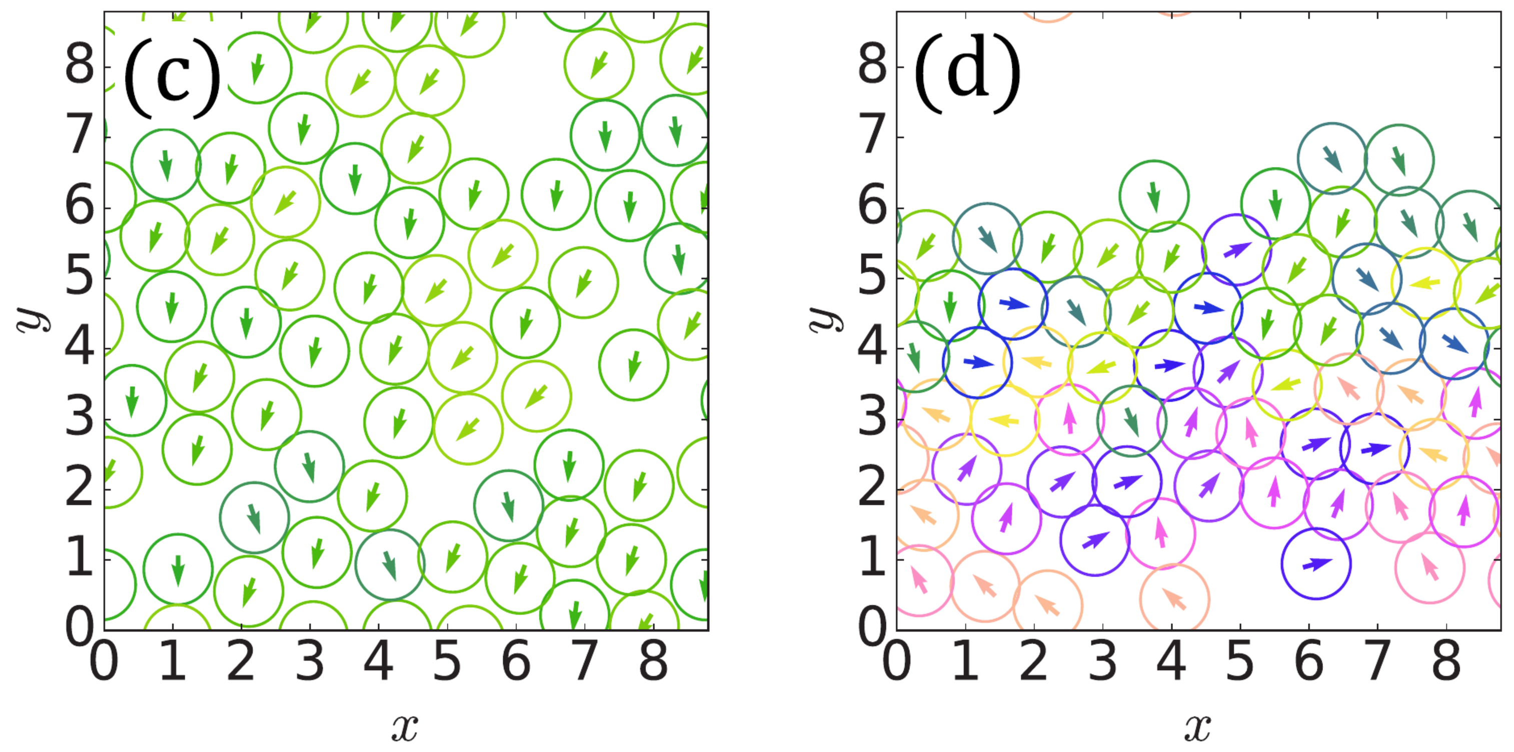


Fig.: Snapshots (Ref. [1], Fig. 1(c,d)) in the collective motion (CM) and phase separated arrested (PSA) phases. Arrows and colors encode the direction of self-propulsion.

Model and methods

Natural dynamics

N ABPs in 2D, with diameters σ, positions $\boldsymbol{r}_i$ and orientations $\boldsymbol{u}_i \equiv (\cos\theta_i, \sin\theta_i)$, interacting via a WCA potential U, following

$$\dot{\boldsymbol{r}}_i = v_0\boldsymbol{u}_i - D\nabla_i U + \sqrt{2D}\,\boldsymbol{\eta}_i$$
$$\dot{\theta}_i = \sqrt{2D_r}\,\xi_i$$

with $\boldsymbol{\eta}_i$, ξ_i Gaussian white noises, in a square box with periodic boundary conditions, at packing fraction $\phi = 0.65$. Ratio $\tilde{l}_{\mathrm{p}} = v_0/\sigma D_r$ is the scaled persistence length.

Orientational order parameter

An **orientational order parameter** (polarisation) quantifies collective motion

$$\boldsymbol{\nu} = \frac{1}{N}\sum_{i=1}^{N}\boldsymbol{u}_i,\ \nu = |\boldsymbol{\nu}|,\ \bar{\nu}_\tau = \frac{1}{\tau}\int_0^\tau \nu(t)\,\mathrm{d}t.$$

Active work

We use a dimensionless and normalised measure of the work of non-conservative self-propulsion forces

$$w_\tau = \frac{1}{v_0 N\tau}\sum_{i=1}^{N}\int_0^\tau \boldsymbol{u}_i \circ \mathrm{d}\boldsymbol{r}_i$$

called **active work**, illustrated thereafter.

Biased ensemble

Active work w_τ satisfies a **large deviation principle** in the limit of large τ

$$P(w_\tau) \asymp \exp[-\tau N I(w_\tau)]$$

where $I(w_\tau)$ is a scaled **rate function**, which is related to the scaled cumulant generating function

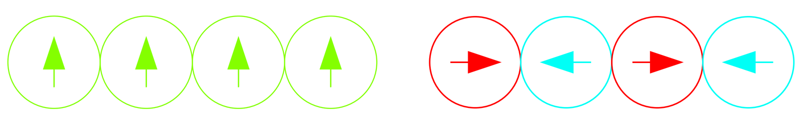
$$\psi(s) = \lim_{\tau\to\infty}\frac{1}{N\tau}\log\left\langle\exp\left(-sN\tau w_\tau\right)\right\rangle$$

via Legendre transform, where s is the **biasing parameter**. A Boltzmann-like distribution of trajectories is defined, with respect to which the **biased average** of an observable $\mathcal{A}$ is

$$\langle\mathcal{A}\rangle_s = \frac{\left\langle\mathcal{A}\,e^{-sN\tau w_\tau}\right\rangle}{\left\langle e^{-sN\tau w_\tau}\right\rangle}$$

and is computed numerically with a **cloning algorithm**.

Flocking | **Jamming**



$\boldsymbol{u}_i \cdot \nabla_i U = 0$, $w_\tau \approx 1, \nu = 1$ | $\dot{\boldsymbol{r}}_i \approx 0$, $w_\tau \approx 0, \nu = 0$

Transition to collective motion

- **Dynamical phase transition** between an isotropic ($\langle\bar{\nu}_\tau\rangle_s = \mathcal{O}(1/N)$) and a CM state ($\langle\bar{\nu}_\tau\rangle_s = \mathcal{O}(1)$) at $s^* \approx -D_r$, $\langle w_\tau\rangle_{s^*} = w^*$, denoted by the maximum in
$$-\partial_s\langle w_\tau\rangle_s = \partial_s^2\psi(s) = \lim_{\tau\to\infty}\tau N \mathrm{Var}(w_\tau)_s.$$

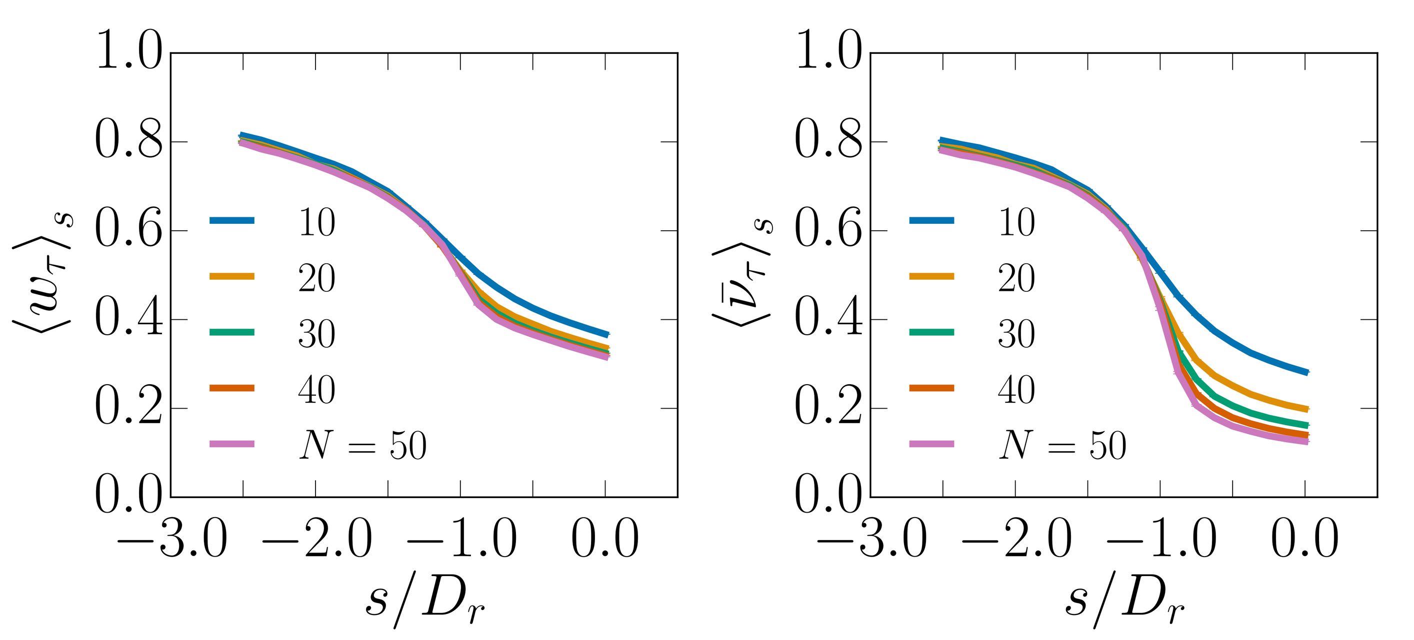


Fig.: Biased averages of the active work $\langle w_\tau\rangle_s$ and the orientational order parameter $\langle\bar{\nu}_\tau\rangle_s$ as functions of the biasing parameter s at $\tilde{l}_{\mathrm{p}} = 5$.

Collective motion state

Modified orientational dynamics
$$\dot{\theta}_i = -D_r\frac{\partial}{\partial\theta_i}\left(-\frac{gN}{D_r}\nu^2\right) + \sqrt{2D_r}\xi_i$$
give an **upper bound** to the rate function
$$I(\langle w_\tau\rangle_g^{\mathrm{con}}) \leq \lim_{\tau\to\infty}\frac{1}{N\tau}\left\langle\log P_g^{\mathrm{con}}/P\right\rangle_g^{\mathrm{con}}.$$

Contraction principle gives a **lower bound** to the rate function
$$I(\langle w_\tau\rangle_s) \geq \mathcal{J}_1(\langle\bar{\nu}_\tau\rangle_s)$$
from $\mathcal{J}_1$ the rate function of polarisation ν.

- In the CM state ($w > w^*$) both bounds perform well, showing that **fluctuations of w_τ are strongly coupled to those of $\bar{\nu}_\tau$**.

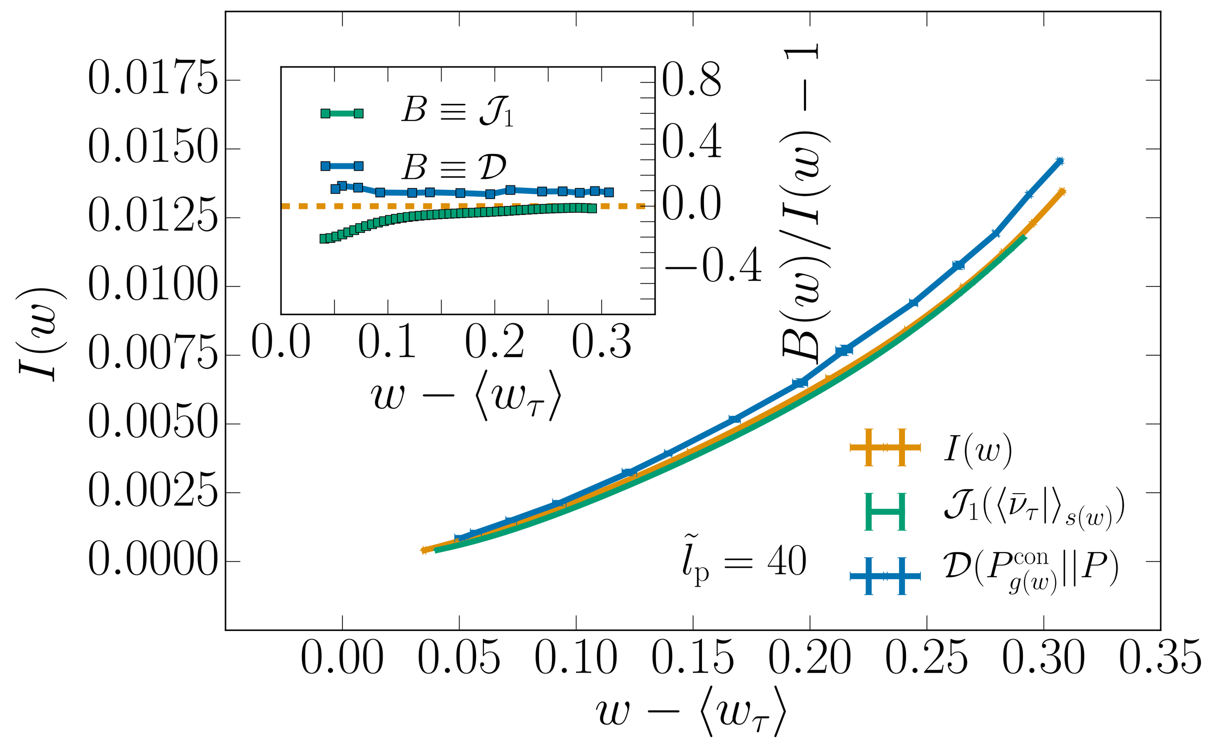


Fig.: Rate function $I(w)$ (orange) with upper bound from controlled dynamics (blue) and lower bound from the cloning of rotors (green). Inset shows the relative errors of these bounds to the rate function.

Hydrodynamic description

Consider a **minimal top-down hydrodynamic description** of ABPs
$$\dot{\rho} = -\nabla\cdot\left(v_0\rho\boldsymbol{P} - D(\rho)\nabla\rho + \sqrt{2\sigma(\rho)}\boldsymbol{\eta}\right),$$
$$\dot{\boldsymbol{P}} = -\gamma(\rho,\boldsymbol{P})f(\boldsymbol{P}) + b(\rho,\boldsymbol{P})\nabla\rho + \sqrt{2\gamma(\rho,\boldsymbol{P})}\boldsymbol{\xi}.$$

Laudau theory

Typical behaviour in the biased ensemble is obtained by **minimising the action**
$$\mathcal{S} = \frac{L^2}{D(\bar{\rho})}\left[\bar{\rho}\mathcal{J}(\boldsymbol{P}) + s\bar{\rho}\left(\langle w_\tau\rangle + \frac{c_\omega}{2}|\boldsymbol{P}|^2\right)\right]$$
with $\mathcal{J}$ the rate function of polarisation $\boldsymbol{\nu}$.

- It predicts a **spontaneous breaking of symmetry** at $s^* = -D_r/c_\omega \approx D_r$.

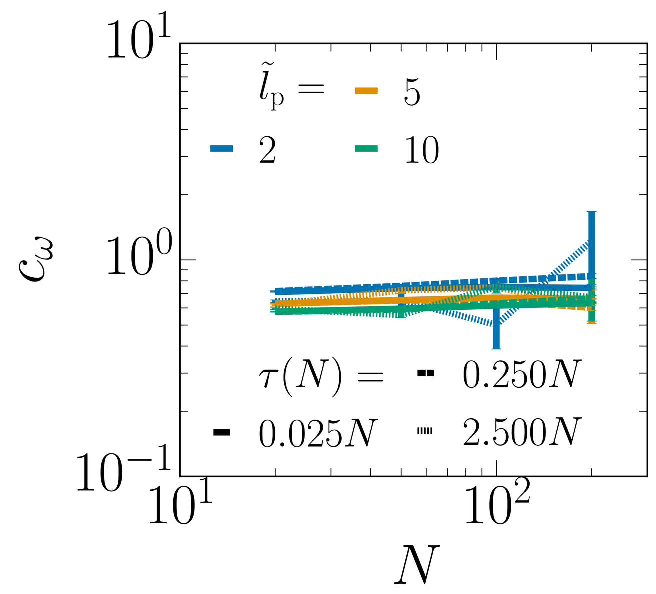


Fig.: Covariance $c_\omega = \frac{\bar{\rho}\tau^2L^4D_r^2}{2}\mathrm{Cov}\left(w_\tau, |\boldsymbol{\nu}_\tau|^2\right)$.

Density fluctuations

At $\boldsymbol{P} = 0$ it is equivalent to bias with respect to $|\tilde{\rho}_{\boldsymbol{q}}|^2$, and it follows
$$S_s(q) = \langle|\tilde{\rho}_{\boldsymbol{q}}|^2\rangle_s = \begin{cases}\chi_0, & s = 0,\\ b_s q, & s < 0.\end{cases}$$

- In finite simulations, biasing results in a **suppression of density fluctuations**.

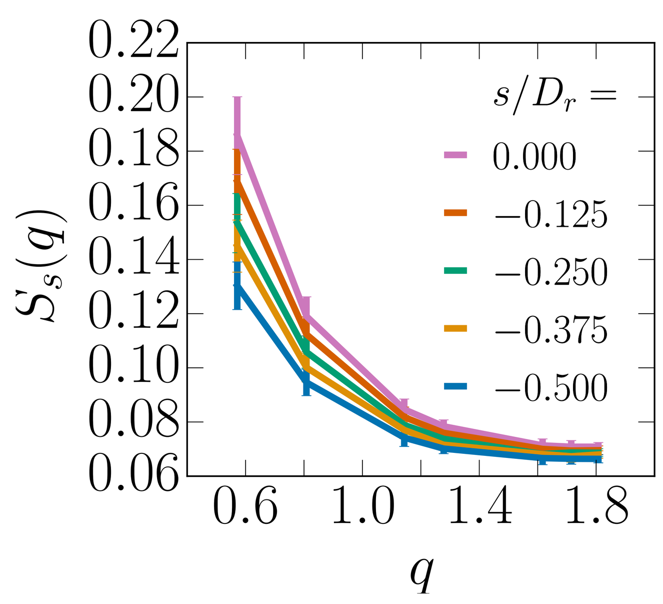


Fig.: Biased structure factor at $\tilde{l}_{\mathrm{p}} = 5$ and $N = 100$.

Conclusions

- Spontaneous breaking of rotational symmetry happens at **finite biasing**, and is qualitatively understood through the introduction of **effective aligning interactions**.
- In the isotropic regime, enhanced active work is associated with **suppressed density fluctuations**.

References

[1] Nemoto, T., Fodor, É., Cates, M. E., Jack, R. L. & Tailleur, J. Optimizing active work: Dynamical phase transitions, collective motion, and jamming. *Physical Review E* **99**, 022605 (2019).

[2] Keta, Y.-E., Fodor, É., van Wijland, F., Cates, M. E. & Jack, R. L. Collective motion in large deviations of active particles. *arXiv*, 2009.07112 (2020).

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