



Collective motion in large deviations of active particles

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in collaboration with E. Fodor, F. van Wijland, M.E. Cates, and R.L. Jack

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1 Active matter

- Non-equilibrium systems
- Active Brownian particles

2 Large deviation theory

- Concepts and applications
- Biased trajectories and cloning algorithm

3 Dynamical phase transitions for active Brownian particles

4 Collective motion mechanism

- CM transition point
- 2 run-and-tumble particles on a ring
- Hydrodynamic theory

5 Conclusion

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5 Conclusion

Non-equilibrium dynamics breaks time-reversal symmetry and thus detailed balance.

L. Berthier and J. Kurchan, [arXiv preprint arXiv:1906.04039](#) (2019).

M. E. Cates and J. Tailleur, *Annu. Rev. Condens. Matter Phys.* **6**, 219–244 (2015).

Non-equilibrium dynamics breaks time-reversal symmetry and thus detailed balance. We can identify 3 general classes:

- Systems relaxing towards equilibrium.

Example

Thermal system adapting to its thermostat, glasses.

L. Berthier and J. Kurchan, [arXiv preprint arXiv:1906.04039](#) (2019).

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Non-equilibrium dynamics breaks time-reversal symmetry and thus detailed balance. We can identify 3 general classes:

- Systems relaxing towards equilibrium.
- Systems with boundary conditions imposing steady currents.

Example

Sheared liquid, metal rod between two thermostats.

L. Berthier and J. Kurchan, [arXiv preprint arXiv:1906.04039 \(2019\)](#).

M. E. Cates and J. Tailleur, [Annu. Rev. Condens. Matter Phys. 6, 219–244 \(2015\)](#).

Non-equilibrium dynamics breaks time-reversal symmetry and thus detailed balance. We can identify 3 general classes:

- Systems relaxing towards equilibrium.
- Systems with boundary conditions imposing steady currents.
- Active matter.

Definition

System composed of self-driven units, *active particles*, each capable of converting stored or ambient free energy into systematic movement.

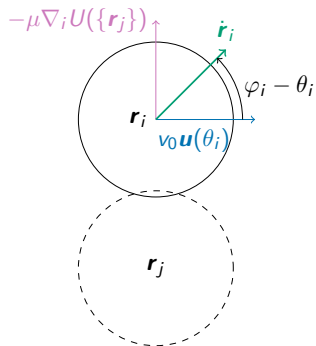
M. C. Marchetti et al., *Reviews of Modern Physics* **85**, 1143 (2013).

Example

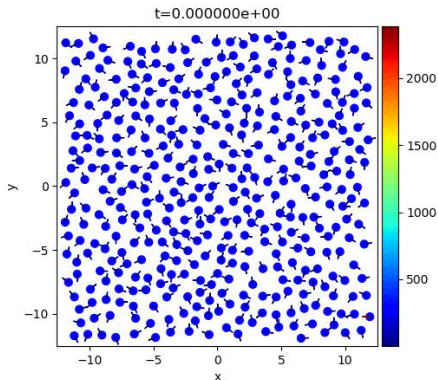
Cell tissues, swarms of bacteria, schools of fish, flocks of birds.

L. Berthier and J. Kurchan, *arXiv preprint arXiv:1906.04039* (2019).

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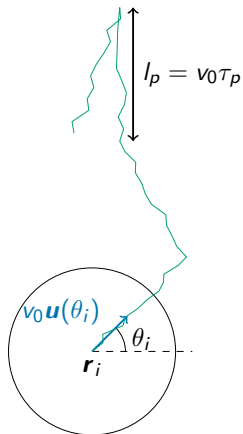


$$\dot{\theta}_i = \frac{1}{\tau_p}(\varphi_i - \theta_i) + \xi_i \quad (1)$$

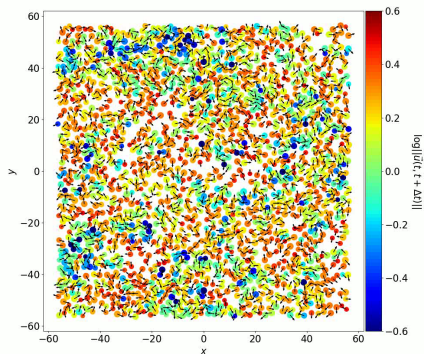


T. Vicsek et al., *Physical Review Letters* **75**, 1226 (1995).

B. Szabo et al., *Physical Review E* **74**, 061908 (2006).



$N = 2.00e + 03, \phi = 0.50, \tilde{v} = 1.00e - 02, \tilde{v}_r = 5.00e - 06, L = 1.128e + 02$
 $t = 0.00000e + 00, \Delta t = 5.00000e + 02$



$$\dot{\theta}_i = \sqrt{2\tau_p^{-1}}\xi_i \quad (2)$$

$$\langle \mathbf{u}(\theta_i(0)) \cdot \mathbf{u}(\theta_i(t)) \rangle = e^{-t/\tau_p} \quad (3)$$

M. E. Cates and J. Tailleur, *Annu. Rev. Condens. Matter Phys.* **6**, 219–244 (2015).

Y.-E. Keta and J. Rottler, *EPL (Europhysics Letters)* **125**, 58004 (2019).

$$\dot{\mathbf{r}}_i = -\mu \nabla_i U(\{\mathbf{r}_j\}) + v_0 \mathbf{u}(\theta_i) + \sqrt{2D} \boldsymbol{\eta}_i \quad (4)$$

$$\dot{\theta}_i = \sqrt{2D_r} \xi_i \quad (5)$$

T. Nemoto et al., *Physical Review E* **99**, 022605 (2019).

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7 control parameters: $N, \phi, \sigma, \mu, v_0, D, D_r$.

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5 control parameters: N , ϕ , μ , D , D_r .

→ Units of space and time: $\sigma = 1$, $\sigma/v_0 = 1$.

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4 control parameters: N , ϕ , μ , $\tilde{l}_p = D_r^{-1}$.

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→ Stokes-Einstein relation: $D = \frac{1}{3} D_r = \frac{1}{3} \tilde{l}_p^{-1}$.

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- Units of space and time: $\sigma = 1$, $\sigma/v_0 = 1$.
- Stokes-Einstein relation: $D = \frac{1}{3}D_r = \frac{1}{3}\tilde{l}_p^{-1}$.
- Scaling of energy: $\mu = D$.

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$$\text{EOM} \quad \dot{\mathbf{r}}_i = v_0 \mathbf{u}(\theta_i) - D \nabla_i U + \sqrt{2D} \boldsymbol{\eta}_i \quad (6)$$

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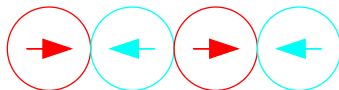
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Flocking



$$\mathbf{u}(\theta_i) \cdot \nabla_i U = 0 \Rightarrow \langle w_\tau \rangle = 1$$

Jamming



$$\dot{\mathbf{r}}_i = 0 \Rightarrow \langle w_\tau \rangle = 0$$

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X_1, \dots, X_n a sequence of (i.i.d.) random variables

$$\langle X_i \rangle = \mu, \quad \langle (X_i - \mu)^2 \rangle = \sigma^2 \quad (11)$$

$$\text{sample average } R_n = \frac{1}{n} \sum_{i=1}^n X_i \quad (12)$$

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Law of large numbers

$$P \left(\lim_{n \rightarrow \infty} R_n = \mu \right) = 1 \quad (13)$$

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Central limit theorem

$$P(R_n) \underset{n \rightarrow \infty}{\sim} \mathcal{N} \left(\mu, \frac{\sigma^2}{n} \right) \quad (13)$$

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Large deviation principle

$$R_n \text{ satisfies a LDP } \Leftrightarrow -\log P(R_n = r) \underset{n \rightarrow \infty}{\sim} nI(r) \quad (13)$$

$$I \equiv \text{rate function of } R_n \Leftrightarrow P(R_n = r) \asymp \exp(-nI(r)) \quad (14)$$

X_1, \dots, X_n random bits, taking value 0 or 1 with equal probability

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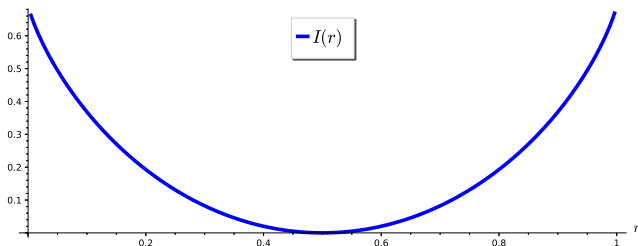
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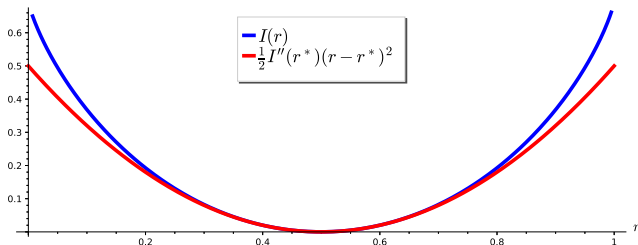


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Gärtner-Ellis theorem

$$\psi \text{ is differentiable} \Rightarrow I(r) = \sup_s \{-sr - \psi(s)\} \quad (19)$$

mean energy per particle for n particles E_n

$$\text{Boltzmann distribution } P_\beta(\omega) = \frac{e^{-\beta n E_n(\omega)}}{Z_n(\beta)} \quad (20)$$

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$$\begin{aligned} \text{SCGF } \psi_\beta(\Delta\beta) &= \lim_{n \rightarrow \infty} \frac{1}{n} \log \int e^{-\Delta\beta n E_n(\omega)} P_\beta(\omega) d\omega \\ &= \lim_{n \rightarrow \infty} \frac{1}{n} \log \frac{Z_n(\beta + \Delta\beta)}{Z_n(\beta)} \\ &= \beta F(\beta) - (\beta + \Delta\beta) F(\beta + \Delta\beta) \end{aligned} \quad (21)$$

$$\text{free energy density } \beta F(\beta) = - \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_n(\beta) \quad (22)$$

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$$I_\beta(E_n) = 0 \Leftrightarrow F(\beta) = E_n - \frac{1}{\beta} S(E_n) \quad (26)$$

d -dimensional system of size N represented by $\{\mathbf{X}_1(t), \dots, \mathbf{X}_N(t)\}$

$$R_{N\tau} = \frac{1}{N\tau} \int_0^\tau \sum_{i=1}^N f(\mathbf{X}_i(t)) dt \quad (27)$$

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Quantity	Equilibrium counterpart	
$\{\mathbf{X}_i(t)\}$	ω	Microstate in $(d+1)$ -dim.
$R_{N\tau}$	E_n	Mean energy
s	$\Delta\beta$	Inverse temperature
ψ	$\beta F(\beta) - (\beta + \Delta\beta)F(\beta + \Delta\beta)$	Free energy
I	$-S(E_n) + \beta E_n - \beta F(\beta)$	Entropy

equilibrium **canonical ensemble** \rightarrow **biased ensemble** of trajectories

$$P_s[\{\mathbf{X}_i(t)\}] \propto P_0[\{\mathbf{X}_i(t)\}] e^{-s N_\tau R_{N_\tau}} \quad (29)$$

$$\langle \mathcal{A} \rangle_s = \frac{\langle \mathcal{A} e^{-s N_\tau R_{N_\tau}} \rangle}{\langle e^{-s N_\tau R_{N_\tau}} \rangle} \quad (30)$$

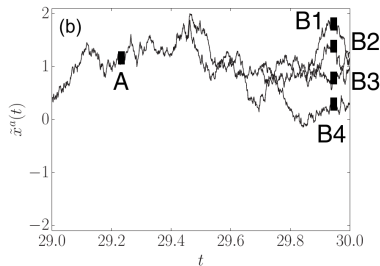
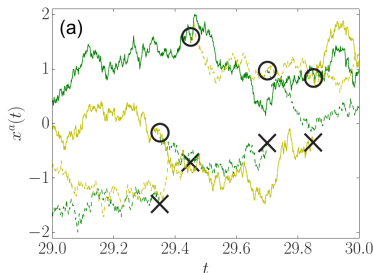
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$$\psi(s) = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \log \left\langle e^{s \int_0^\tau x(t)(1+x(t)) dt} \right\rangle \quad (31)$$

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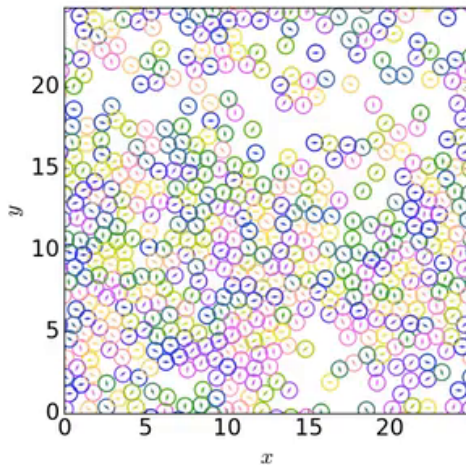
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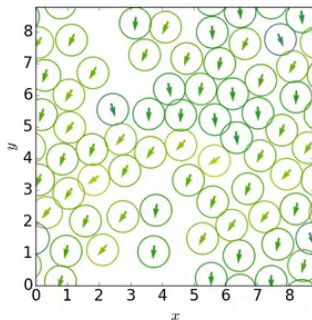
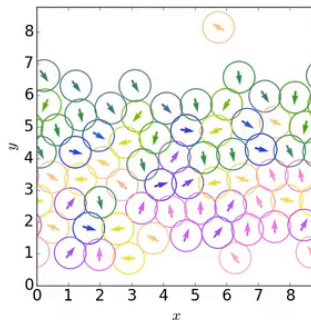
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- 3 Description of qualitative changes at dynamical transition.



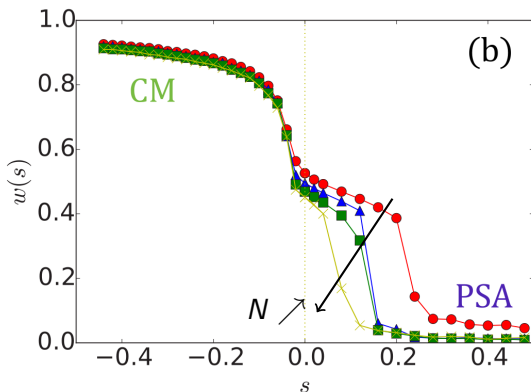
T. Nemoto et al., *Physical Review E* 99, 022605 (2019).

CM ($s < 0$)PSA ($s > 0$)

CM \equiv collective motion, PSA \equiv phase-separated arrest

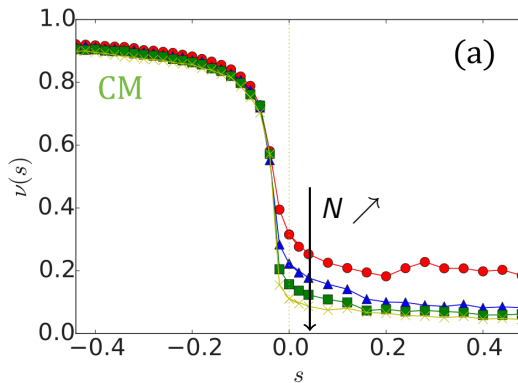
$$\langle w_\tau \rangle_s = w(s) = -\psi'(s) \quad (32)$$

$$-w'(s) = \psi''(s) = \lim_{\tau \rightarrow \infty} N\tau \text{Var}(w_\tau)_s \quad (33)$$



$$\text{polarisation } \hat{\nu} = \left| \frac{1}{N} \sum_{i=1}^N \mathbf{u}(\theta_i) \right|, \quad \bar{\nu}_\tau = \frac{1}{\tau} \int_0^\tau \hat{\nu}(t) dt \quad (34)$$

$$\langle \bar{\nu}_\tau \rangle = \langle \bar{\nu}_\tau \rangle_{s=0} \propto N^{-1/2} \quad (35)$$



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- Non-equilibrium systems
- Active Brownian particles

2 Large deviation theory

- Concepts and applications
- Biased trajectories and cloning algorithm

3 Dynamical phase transitions for active Brownian particles

4 Collective motion mechanism

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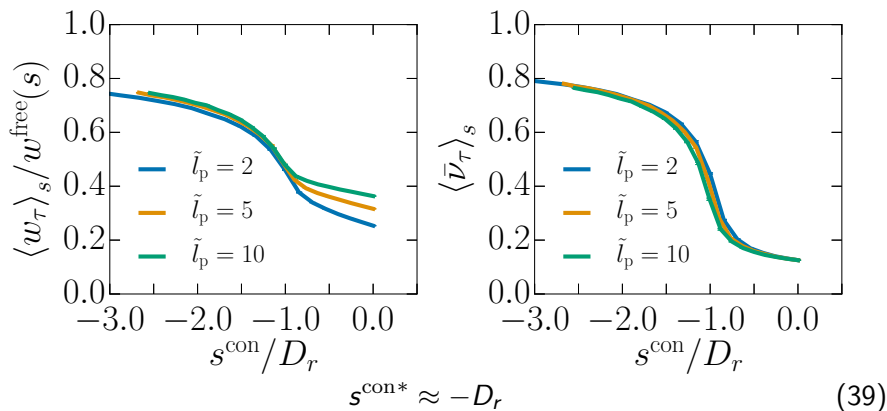
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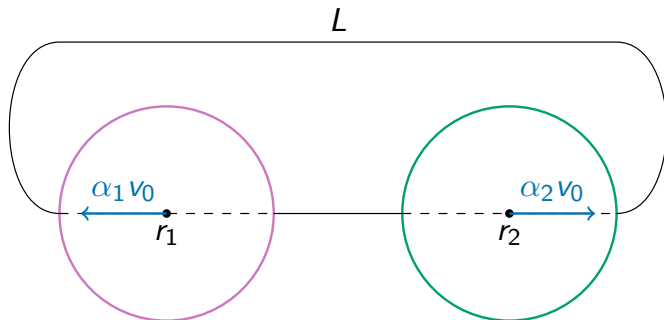
$$s^* \neq 0 \Rightarrow l \neq 0 \quad (36)$$

- 2 Analytical illustration of collective motion.
- 3 Top-down hydrodynamic description.

$$w^{\text{free}}(s) = 1 - \frac{2sD}{v_0^2} \quad (37)$$

$$s^{\text{con}} = s \left(1 - \frac{2sD}{v_0^2} \right) \quad (38)$$





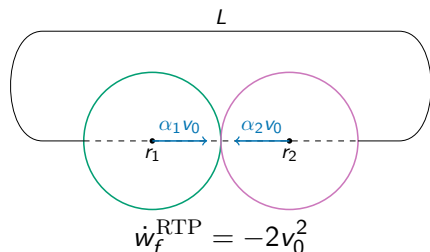
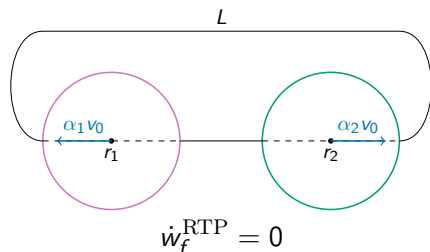
$$\alpha_i \in \{-1, +1\} \quad (40)$$

$$l = \tau_p(\alpha_i \rightarrow -\alpha_i) v_0 \quad (41)$$

A. Slowman et al., *Physical Review Letters* **116**, 218101 (2016).

F. Cagnetta and E. Mallmin, *Physical Review E* **101**, 022130 (2020).

$$\text{active work } \dot{w}_f^{\text{RTP}} = v_0(\alpha_1 - \alpha_2)\partial_{r_1} V(r_{12}) \quad (42)$$



$$\text{SCGF} \quad \psi^{\text{RTP}}(\lambda) = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \log \left\langle e^{-\lambda \int_0^\tau \dot{w}_f^{\text{RTP}}(t) dt} \right\rangle \quad (43)$$

$$\text{polarisation} \quad \nu^{\text{RTP}} = \frac{1 + \alpha_1 \alpha_2}{2} \quad (44)$$

$$\psi^{\text{RTP}}(\lambda) \mathbf{P}_\lambda = (\mathcal{L} - \lambda \dot{w}_f^{\text{RTP}}) \mathbf{P}_\lambda \quad (45)$$

$$\mathbf{P}_\lambda(r \equiv r_2 - r_1) \equiv (P_\lambda^{++}(r), P_\lambda^{--}(r), P_\lambda^{+-}(r), P_\lambda^{-+}(r)) \quad (46)$$

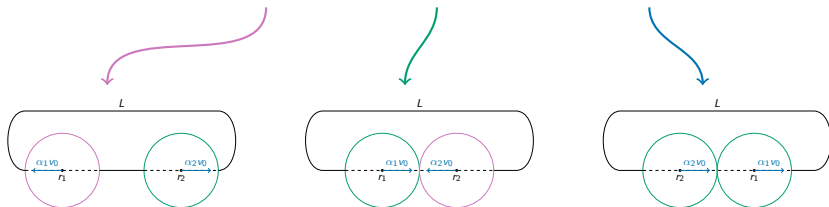
H. Touchette, *Physica A: Statistical Mechanics and its Applications* **504**, 5–19 (2018).

T. Arnoulx de Pirey et al., *Physical Review Letters* **123**, 260602 (2019).

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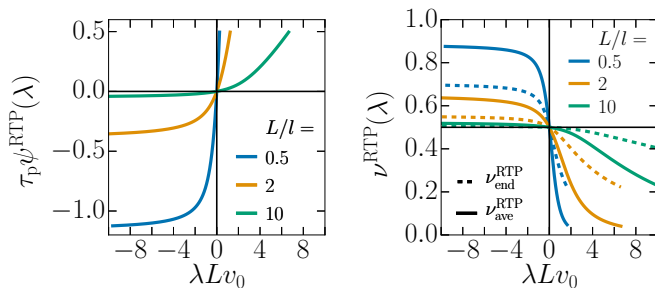
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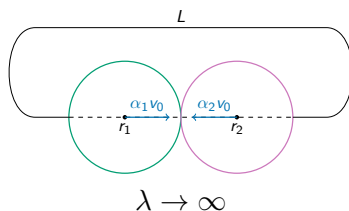
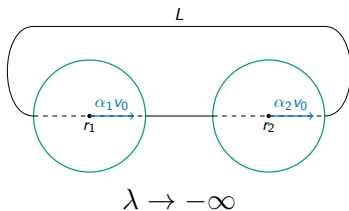


H. Touchette, *Physica A: Statistical Mechanics and its Applications* **504**, 5–19 (2018).

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$$\langle w_f^{\text{RTP}} \rangle_\lambda = -\partial_\lambda \psi^{\text{RTP}}, \quad \nu^{\text{RTP}} = \frac{1 + \alpha_1 \alpha_2}{2} \quad (48)$$



M. E. Cates and J. Tailleur, *EPL (Europhysics Letters)* **101**, 20010 (2013).

M. E. Cates, *arXiv preprint arXiv:1904.01330* (2019).

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$$S = \frac{D}{4\sigma} |\mathbf{J} - \mathbf{J}_d|^2 + \frac{1}{4D\gamma} \left| \frac{D}{L} \dot{\mathbf{P}} + \gamma \mathbf{f}L - b \nabla \rho \right|^2 + \frac{sL^2}{D} \omega \quad (59)$$

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$$\text{LDP on polarisation } P_{s=0}[\bar{\rho}, \mathbf{J}_d, \mathbf{P}] \propto \exp\left(-\frac{L^2 t}{D} \bar{\rho} \mathcal{J}(\mathbf{P})\right) \quad (61)$$

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$$S = \frac{\bar{\rho} L^2}{D} \left[s \langle w_{\tau} \rangle + \frac{1}{2} (D_r + s c_{\omega}) |\mathbf{P}|^2 + \mathcal{O}(|\mathbf{P}|^4) \right] \quad (60)$$

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N. Goldenfeld, (CRC Press, 2018).

Y.-E. Keta et al., *Physical Review E* 103, 022603 (2021).

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analogy with a **ferromagnet**

$$\mathcal{L}(H = 0) = a(T_c)(T - T_c)\eta^2 + \mathcal{O}(\eta^4), \quad T_c \propto J \quad (65)$$

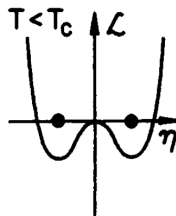
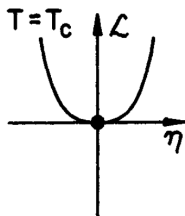
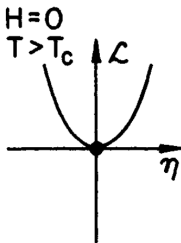
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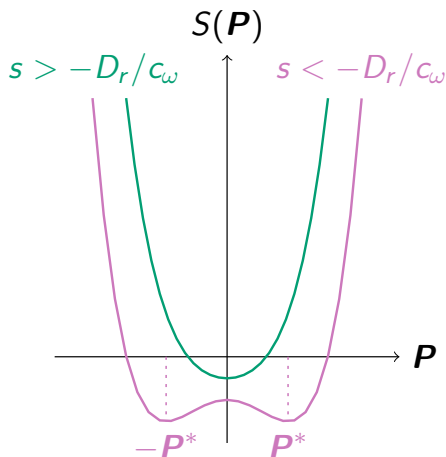
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- We have proposed a **fluctuating hydrodynamic theory** which captures the emergence of polar order in the biased state.

Thank you!

→ In the s -ensemble of trajectories $x(0 \leq t \leq \tau)$, $t = 0$ and $t = \tau$ are boundaries \Rightarrow dynamical analogue of boundary effects.

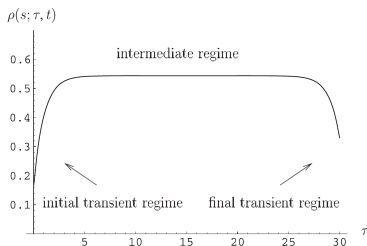


Figure: [from: J. P. Garrahan et al., *Journal of Physics A: Mathematical and Theoretical* **42**, 075007 (2009) (Fig. 7)]

$$P_{\text{end}}(x) = \lim_{\tau \rightarrow \infty} \langle \delta(x(\tau) - x) \rangle_s \quad (65)$$

$$P_{\text{ave}}(x) = \lim_{\tau \rightarrow \infty} \left\langle \tau^{-1} \int_0^\tau \delta(x(t) - x) dt \right\rangle_s \quad (66)$$

$$\text{SDE} \quad \dot{\mathbf{X}} = F(\mathbf{X}) + \sqrt{2D}\boldsymbol{\eta} \quad (67)$$

$$\text{Fokker-Planck equation} \quad \frac{\partial}{\partial t} P(\mathbf{x}, t) = \mathcal{L}P(\mathbf{x}, t) \quad (68)$$

$$P(\mathbf{x}, t) = P(\mathbf{X}(t) = \mathbf{x}) \quad (69)$$

$$\text{observable} \quad A_\tau = \frac{1}{\tau} \int_0^\tau f(\mathbf{X}(t)) \, dt \quad (70)$$

$$\text{SCGF} \quad \psi(s) = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \log \langle \exp(-s\tau A_\tau) \rangle \quad (71)$$

→ $\psi(s)$ is the largest eigenvalue of $\mathcal{L} - sf$.

$$\lambda(s)l(\mathbf{x}) = (\mathcal{L} - sf(\mathbf{x}))l(\mathbf{x}) \quad (72)$$

$$P_{\text{end}}(\mathbf{x}) = l(\mathbf{x}) \quad (73)$$

$$\lambda(s)r(\mathbf{x}) = (\mathcal{L}^\dagger - sf(\mathbf{x}))r(\mathbf{x}) \quad (74)$$

$$P_{\text{ave}}(\mathbf{x}) = l(\mathbf{x})r(\mathbf{x}) \quad (75)$$

“Large deviations occur according to the least unlikely mechanism.”

$$I_A(w) \leq I(w) \leq I_B(w) \text{ the closer the better} \quad (76)$$

$$\dot{\mathbf{r}}_i = \mathbf{v}_s^{\text{con}} \mathbf{u}(\theta_i) - D \nabla_i U + \sqrt{2D} \boldsymbol{\eta}_i \quad (77)$$

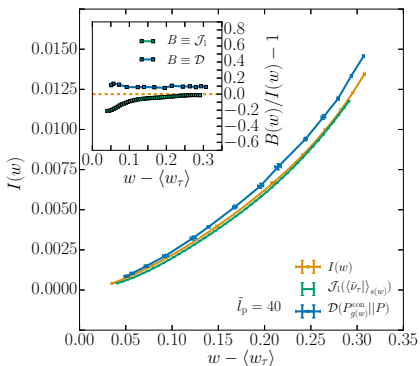
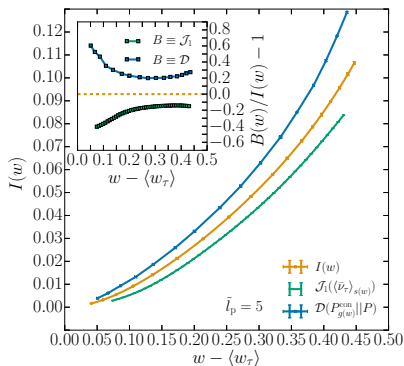
$$\dot{\theta}_i = -D_r \frac{\partial}{\partial \theta_i} U_g^{\text{con}} + \sqrt{2D_r} \xi_i \quad (78)$$

$$I(w) \leq \lim_{\tau \rightarrow \infty} \mathcal{D}_{\text{KL}}(P_{g(w)}^{\text{mod}} || P) \quad (79)$$

$$\mathcal{D}_{\text{KL}}(P_{g(w)}^{\text{mod}} || P) = \left\langle \log P_{g(w)}^{\text{mod}} / P \right\rangle_{\text{mod}} = f[\{\theta_i(t)\}, g(w)] \quad (80)$$

$$I_{h(A)}(b) = \inf_{a:h(a)=b} I_A(a) \quad (81)$$

$$I(w) \stackrel{\text{CP}}{=} \inf_{\nu} I_2(w, \nu) = I_2(w, \nu(w)) \geq \inf_{w'} I_2(w', \nu(w)) \stackrel{\text{CP}}{=} \mathcal{J}_1(\nu(w)) \quad (82)$$

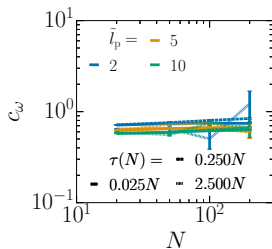


$$\omega(\bar{\rho}, \mathbf{P}) = \langle \bar{\rho} w_\tau \rangle_{\mathbf{h}(\mathbf{P})} = \frac{\langle \bar{\rho} w_\tau \exp(-\tau N \mathbf{h}(\mathbf{P}) \cdot \bar{\mathbf{v}}_\tau) \rangle}{\langle \exp(-\tau N \mathbf{h}(\mathbf{P}) \cdot \bar{\mathbf{v}}_\tau) \rangle} \quad (83)$$

$$\bar{\mathbf{v}}_\tau = \frac{1}{\tau} \int_0^\tau \frac{1}{N} \sum_{i=1}^N \mathbf{u}(\theta_i(t)) dt, \quad \langle \bar{\mathbf{v}}_\tau \rangle_{\mathbf{h}(\mathbf{P})} = \mathbf{P} \quad (84)$$

$$\omega(\bar{\rho}, \mathbf{P}) = \bar{\rho} \left[\langle w_\tau \rangle + \frac{c_\omega}{2} |\mathbf{P}|^2 + \mathcal{O}(|\mathbf{P}|^4) \right] \quad (85)$$

$$c_\omega = \frac{\bar{\rho} \tau^2 L^4 D_r^2}{2} \text{Cov}(w_\tau, |\bar{\mathbf{v}}_\tau|^2) \quad (86)$$



- At $\mathbf{P} = 0$, biasing w.r.t. w_τ is equivalent to biasing w.r.t. $|\tilde{\rho}_\mathbf{q}|^2$.

$$S_s(\mathbf{q}) = \langle |\tilde{\rho}_\mathbf{q}|^2 \rangle_s = \begin{cases} \chi_0, & s = 0 \\ b_s q, & s < 0 \end{cases} \quad (87)$$

⇒ We expect hyperuniformity in the isotropic $s < 0$ phase for $N \gg 1$.

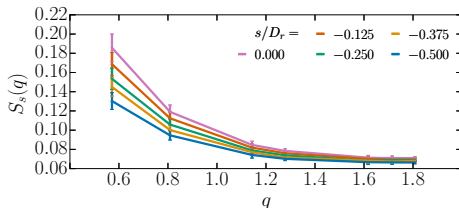


Figure: Biased structure factor S_s .

→ Finite system shows suppression of density fluctuations for $s < 0$.