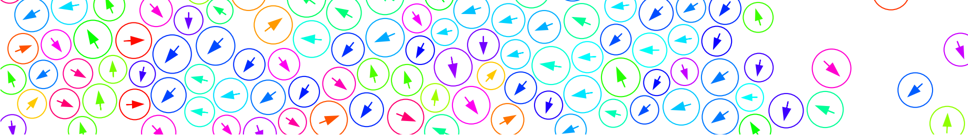


Large deviations of active work in systems of active Brownian particles

Yann-Edwin Keta

supervised by Robert Jack

StatMech meeting, Department of Chemistry,
University of Cambridge

20/02/2020

yketa/DAMTP_MSC_2019_Wiki

UNIVERSITY OF CAMBRIDGE

ENS DE LYON

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

Ludovic Berthier and Jorge Kurchan. "Lectures on non-equilibrium active systems". In: *arXiv preprint arXiv:1906.04039* (2019).

Michael E Cates and Julien Tailleur. "Motility-induced phase separation". In: *Annu. Rev. Condens. Matter Phys.* 6.1 (2015), pp. 219–244.

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.

Ludovic Berthier and Jorge Kurchan. "Lectures on non-equilibrium active systems". In: *arXiv preprint arXiv:1906.04039* (2019).

Michael E Cates and Julien Tailleur. "Motility-induced phase separation". In: *Annu. Rev. Condens. Matter Phys.* 6.1 (2015), pp. 219–244.

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.

Ludovic Berthier and Jorge Kurchan. "Lectures on non-equilibrium active systems". In: *arXiv preprint arXiv:1906.04039* (2019).

Michael E Cates and Julien Tailleur. "Motility-induced phase separation". In: *Annu. Rev. Condens. Matter Phys.* 6.1 (2015), pp. 219–244.

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 Cristina Marchetti et al. "Hydrodynamics of soft active matter". In: *Reviews of Modern Physics* 85.3 (2013), p. 1143.

Example

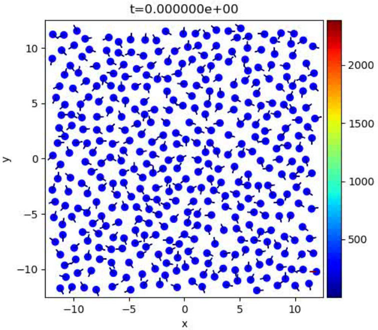
Cell tissues, swarms of bacteria, schools of fish, flocks of birds.

Ludovic Berthier and Jorge Kurchan. "Lectures on non-equilibrium active systems". In: *arXiv preprint arXiv:1906.04039* (2019).

Michael E Cates and Julien Tailleur. "Motility-induced phase separation". In: *Annu. Rev. Condens. Matter Phys.* 6.1 (2015), pp. 219–244.

→ Aligning self-propelled disks with repulsive interactions (Vicsek model).

$$\dot{\underline{r}}_i = v_0 \begin{pmatrix} \cos\theta_i \\ \sin\theta_i \end{pmatrix} - \mu \sum_{j=1}^{N} \nabla U_{ij}, \;\; \dot{\theta}_i = \frac{1}{\tau}(\varphi_i - \theta_i) + \xi_i, \;\; \varphi_i = \arg(\dot{\underline{r}}_i)$$

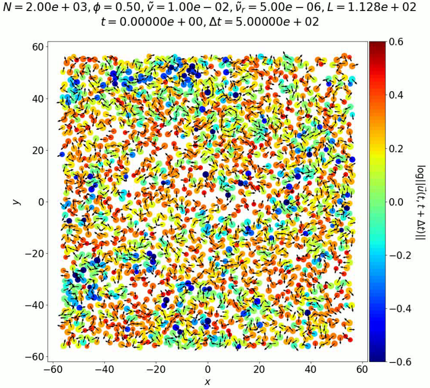


Tamás Vicsek et al. "Novel type of phase transition in a system of self-driven particles". In: *Physical review letters* 75.6 (1995), p. 1226.

Balint Szabo et al. "Phase transition in the collective migration of tissue cells: experiment and model". In: *Physical Review E* 74.6 (2006), p. 061908.

→ Active Brownian particles with repulsive soft interactions.

$$\underline{\dot{r}}_i = v_0 \begin{pmatrix} \cos\theta_i \\ \sin\theta_i \end{pmatrix} - \mu \sum_{j=1}^{N} \nabla U_{ij}, \;\; \dot{\theta}_i = \sqrt{2\tau^{-1}}\xi_i$$



Yann-Edwin Keta and Jörg Rottler. "Cooperative motion and shear strain correlations in dense 2D systems of self-propelled soft disks". In: *EPL (Europhysics Letters)* 125.5 (2019), p. 58004.

→ For $\{\underline{r}_i, \underline{u}_i\}_0^\tau$ a translational and orientational trajectory...

$$\dot{\mathcal{S}}_N\left[\{\underline{r}_i, \underline{u}_i\}_0^\tau\right] = \frac{1}{\tau}\log\frac{\mathcal{P}_N\left[\{\underline{r}_i, \underline{u}_i\}_0^\tau\right]}{\mathcal{P}_N^R\left[\{\underline{r}_i, \underline{u}_i\}_0^\tau\right]},$$

$$\dot{\mathcal{S}}_N = \lim_{\tau\to\infty}\left\langle \dot{\mathcal{S}}_N\left[\{\underline{r}_i, \underline{u}_i\}_0^\tau\right]\right\rangle,$$

→ ... defines a distance to equilibrium which cancels at equilibrium.

$$\dot{\mathcal{S}}_N\left[\{\underline{r}_i, \underline{u}_i\}_0^\tau\right] \propto \frac{1}{\tau}\Delta F \Rightarrow \dot{\mathcal{S}}_N = 0.$$

Étienne Fodor et al. "How far from equilibrium is active matter?" In: *Physical review letters* 117.3 (2016), p. 038103.

Cesare Nardini et al. "Entropy production in field theories without time-reversal symmetry: quantifying the non-equilibrium character of active matter". In: *Physical Review X* 7.2 (2017), p. 021007.

→ N ABPs with evolution

$$\dot{\underline{r}}_i = -\mu \sum_{j=1}^{N} \nabla U_{ij} + v_0 \begin{pmatrix} \cos\theta_i \\ \sin\theta_i \end{pmatrix} + \sqrt{2D}\underline{\eta}_i,$$

$$\dot{\theta}_i = \sqrt{2D_r}\xi_i,$$

→ $U_{ij} \equiv$ WCA potential, $\underline{\eta}_i$, $\xi_i \equiv$ Gaussian white noises with unit variance and zero mean, $\sigma \equiv$ diameter, $\phi \equiv$ packing fraction.

Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605.

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7 control parameters: N, ϕ, σ, μ, v_0, D, D_r.

Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605.

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

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

Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605.

→ N ABPs with evolution

$$\dot{\underline{r}}_i = -\mu \sum_{j=1}^{N} \nabla U_{ij} + \begin{pmatrix} \cos\theta_i \\ \sin\theta_i \end{pmatrix} + \sqrt{2D}\underline{\eta}_i,$$

$$\dot{\theta}_i = \sqrt{2\frac{\sigma}{l_p}}\xi_i,$$

→ $U_{ij} \equiv$ WCA potential, $\underline{\eta}_i$, $\xi_i \equiv$ Gaussian white noises with unit variance and zero mean, $\phi \equiv$ packing fraction.

5 control parameters: N, ϕ, μ, D, $\frac{l_p}{\sigma} = D_r^{-1}$.

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

Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605.

→ N ABPs with evolution

$$\dot{\underline{r}}_i = -\mu \sum_{j=1}^{N} \nabla U_{ij} + \begin{pmatrix} \cos\theta_i \\ \sin\theta_i \end{pmatrix} + \sqrt{\frac{2}{3}\frac{\sigma}{l_p}}\underline{\eta}_i,$$

$$\dot{\theta}_i = \sqrt{2\frac{\sigma}{l_p}}\xi_i,$$

→ $U_{ij} \equiv$ WCA potential, $\underline{\eta}_i$, $\xi_i \equiv$ Gaussian white noises with unit variance and zero mean, $\phi \equiv$ packing fraction.

4 control parameters: N, ϕ, μ, $\frac{l_p}{\sigma} = D_r^{-1}$.

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

→ Stokes-Einstein-Debye relation: $D = \frac{1}{3} D_r$

Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605.

→ N ABPs with evolution

$$\underline{\dot{r}}_i = -\frac{1}{3}\frac{\sigma}{l_p}\sum_{j=1}^{N}\nabla U_{ij} + \begin{pmatrix}\cos\theta_i\\ \sin\theta_i\end{pmatrix} + \sqrt{\frac{2}{3}\frac{\sigma}{l_p}}\underline{\eta}_i,$$
$$\dot{\theta}_i = \sqrt{2\frac{\sigma}{l_p}}\xi_i,$$

→ $U_{ij} \equiv$ WCA potential, $\underline{\eta}_i$, $\xi_i \equiv$ Gaussian white noises with unit variance and zero mean, $\phi \equiv$ packing fraction.

3 control parameters: N, ϕ, $\frac{l_p}{\sigma} = D_r^{-1}$.

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

→ Stokes-Einstein-Debye relation: $D = \frac{1}{3}D_r$

→ $\mu = D$

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$$\dot{\mathcal{S}}_N = \lim_{\tau\to\infty} \left\langle \frac{1}{\tau} \log \frac{\mathcal{P}_N\left[\{\underline{r}_i, \underline{u}_i\}_0^\tau\right]}{\mathcal{P}_N^R\left[\{\underline{r}_i, \underline{u}_i\}_0^\tau\right]} \right\rangle = 3\frac{l_p}{\sigma} N \lim_{\tau\to\infty} \langle w_\tau \rangle$$

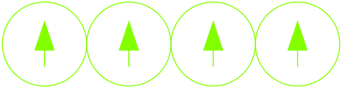
$$w_\tau = \frac{1}{N\tau} \int_0^\tau \sum_{i=1}^N \dot{\underline{r}}_i(t) \cdot \underline{u}(\theta_i(t))\, \mathrm{d}t$$

$$= \frac{1}{N\tau} \int_0^\tau \sum_{i=1}^N \left(1 - \frac{1}{3}\frac{\sigma}{l_p} \sum_{j=1}^N \underline{u}(\theta_i) \cdot \nabla U_{ij} + \sqrt{\frac{2}{3}\frac{\sigma}{l_p}} \underline{u}(\theta_i) \cdot \underline{\eta}_i \right) \mathrm{d}t$$

$$\dot{\mathcal{S}}_N = \lim_{\tau \to \infty} \left\langle \frac{1}{\tau} \log \frac{\mathcal{P}_N\left[\{\underline{r}_i, \underline{u}_i\}_0^\tau\right]}{\mathcal{P}_N^R\left[\{\underline{r}_i, \underline{u}_i\}_0^\tau\right]} \right\rangle = 3\frac{l_p}{\sigma} N \lim_{\tau \to \infty} \langle w_\tau \rangle$$

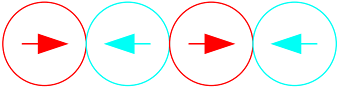
$$\begin{aligned} w_\tau &= \frac{1}{N\tau} \int_0^\tau \sum_{i=1}^N \dot{\underline{r}}_i(t) \cdot \underline{u}(\theta_i(t))\,\mathrm{d}t \\ &= \frac{1}{N\tau} \int_0^\tau \sum_{i=1}^N \left(1 - \frac{1}{3}\frac{\sigma}{l_p} \sum_{j=1}^N \underline{u}(\theta_i) \cdot \nabla U_{ij} + \sqrt{\frac{2}{3}\frac{\sigma}{l_p}}\,\underline{u}(\theta_i) \cdot \underline{\eta}_i\right) \mathrm{d}t \end{aligned}$$

Flocking



$\nabla U_{ij} = 0 \Rightarrow w_\tau \approx 1$

Jamming



$\dot{\underline{r}}_i \approx 0 \Rightarrow w_\tau \approx 0$

→ $X_1, \ldots, X_n$ a sequence of random numbers and its sample average

$$S_n = \frac{1}{n}\sum_{i=1}^{n} X_i.$$

$$S_n \text{ satisfies a LDP } \Leftrightarrow \lim_{n\to\infty} -\frac{1}{n}\log P(S_n = s) = I(s)$$

$$I \equiv \text{ rate function of } S_n \Leftrightarrow P(S_n = s) \asymp \exp(-nI(s))$$

Hugo Touchette. "The large deviation approach to statistical mechanics". In: *Physics Reports* 478.1-3 (2009), pp. 1–69.

$\rightarrow$ $X_1, \dots, X_n$ random numbers from a Gaussian distribution (μ, σ).

$$S_n = \frac{1}{n} \sum_{i=1}^{N} X_i,$$

$$P(S_n = s) = \sqrt{\frac{n}{2\pi\sigma^2}} e^{-n(s-\mu)^2/(2\sigma^2)}.$$

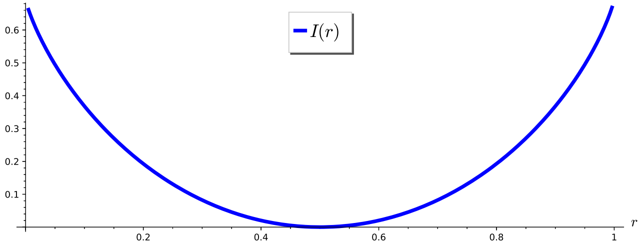
$$\lim_{n\to\infty} -\frac{1}{n} \log P(S_n = s) = (s-\mu)^2/(2\sigma^2) = I(s).$$

$\Rightarrow$ S_n satisfies a large deviation principle.

→ $B_1, \ldots, B_n$ random bits, taking value 0 or 1 with equal probability.

$$R_n = \frac{1}{n}\sum_{i=1}^{n} B_i$$

$$P(R_n = r) \asymp \exp(-nI(r)),\ \ I(r) = \log 2 + r\log r + (1-r)\log(1-r).$$



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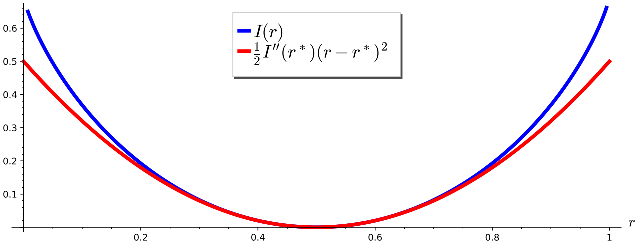

→ Deviations from the Gaussian fluctuations predicted by the Central Limit Theorem ⇒ *large* deviations.

Scaled cumulant generating function (SCGF)

$$\lambda(k) = \lim_{n\to\infty} \frac{1}{n} \log \int e^{nka} P(A_n = a)\, \mathrm{d}a = \lim_{n\to\infty} \frac{1}{n} \log \left\langle e^{nkA_n} \right\rangle .$$

$$\lambda \text{ is differentiable } \Rightarrow I(a) = \sup_k \{ka - \lambda(k)\} = k(a)a - \lambda(k(a))$$

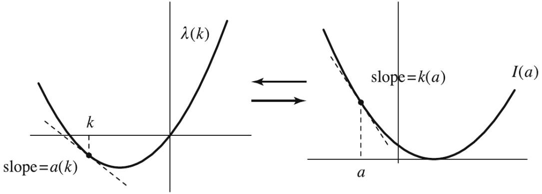

Figure: [from: Hugo Touchette. "The large deviation approach to statistical mechanics". In: *Physics Reports* 478.1-3 (2009), pp. 1–69]

$$E_n \equiv \text{energy of } n \text{ particles} \Rightarrow P_\beta(\omega) = \frac{e^{-\beta n E_n(\omega)}}{Z_n(\beta)} \equiv \text{Boltzmann distribution}$$

$$\begin{aligned}\psi(\Delta\beta) &= \lim_{n\to\infty} \frac{1}{n} \log \int e^{\Delta\beta n E_n(\omega)} P_\beta(\omega)\, \mathrm{d}\omega = \lim_{n\to\infty} \frac{1}{n} \log \frac{Z_n(\beta - \Delta\beta)}{Z_n(\beta)} \\ &= \beta F(\beta) - (\beta - \Delta\beta) F(\beta - \Delta\beta)\end{aligned}$$

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

$$\psi \text{ is differentiable} \xRightarrow[\text{Gärtner-Ellis}]{} P_\beta(E_n) \asymp \exp(-nI_\beta(E_n))$$

$$P_\beta(E_n) \asymp \exp(n(\underbrace{s(E_n)}_{\substack{\text{entropy}\\ \equiv\text{number of states}}} - \overbrace{\beta E_n}^{\substack{\text{Boltzmann}\\ \text{function}}} + \underbrace{\beta F(\beta)}_{\substack{\text{partition}\\ \text{function}}}))$$

$$I_\beta(E_n) = -s(E_n) - \beta E_n + \beta F(\beta)$$

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

→ d-dimensional system of size N, quantities $a_i(t)$ over trajectories.

$$A_{N\tau} = \frac{1}{N\tau}\int_0^\tau \sum_{i=1}^{N} a_i(t)\,\mathrm{d}t$$

$$I_N(a) = \lim_{\tau\to\infty} -\frac{1}{\tau}\log P(A_\tau = a),\ \ \psi_N(s) = \lim_{\tau\to\infty} \frac{1}{\tau}\log\left\langle e^{sN\tau A_\tau}\right\rangle$$

Quantity	Equilibrium counterpart
a_i	Microstates of $(d+1)$-dimensional system
$A_{N\tau}$	Mean energy
s	Inverse temperature (conjugate to the energy)
ψ_N	Free energy difference
I_N	$-s(E_n) - \beta E_n + \beta F(\beta)$

$\rightarrow$ d-dimensional system of size N, quantities $a_i(t)$ over trajectories.

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I_N	$-s(E_n) - \beta E_n + \beta F(\beta)$

$\Rightarrow$ Singularities in I_N/N and ψ_N/N in the limit $\tau\to\infty$ and $N\to\infty$ $\Rightarrow$ *dynamical phase transitions*.

$$Z_\tau(s) = \left\langle e^{sN\tau A_{N\tau}} \right\rangle \equiv \begin{array}{l} \textit{dynamical} \text{ partition function} \\ \text{of a Boltzmann-like measure} \end{array}$$

$\rightarrow$ $s \neq 0 \Rightarrow$ average dominated by trajectories with rare events.

$$Z_\tau(s) = \left\langle e^{sN_\tau A_{N_\tau}} \right\rangle \equiv$$ *dynamical* partition function of a Boltzmann-like measure

$\rightarrow$ $s \neq 0 \Rightarrow$ average dominated by trajectories with rare events.

$\Rightarrow$ *Cloning algorithm* to generate the biased measure.

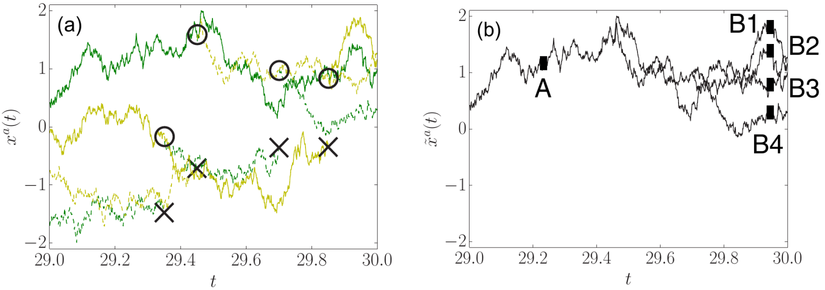

Figure: $Z_\tau(s) = \left\langle \exp\left(s \int_0^\tau x(t)(1 + x(t))\,\mathrm{d}t \right) \right\rangle$. [from: Takahiro Nemoto et al. "Population-dynamics method with a multicanonical feedback control". In: *Physical Review E* 93.6 (2016), p. 062123]

How does the active work (*i.e.* dissipation) control emerging behaviours?

$\Rightarrow$ Cloning algorithm $\rightarrow$ generate trajectories of systems of ABPs where large deviations of the active work are typical.

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$\Rightarrow$ Cloning algorithm $\rightarrow$ generate trajectories of systems of ABPs where large deviations of the active work are typical.

$\rightarrow$ Compute SCGF...

$$\psi_N(s,\tau) = \frac{1}{\tau}\log\left\langle e^{-sN\tau w_\tau}\right\rangle,$$

$$s > 0 \Leftrightarrow \text{large } \textbf{negative} \text{ fluctuations of } w(s)$$

... biased average of the active work...

$$w(s) = \langle w \rangle_s = -\psi_N'(s)/N,$$

... and rate function.

$$I_N(w) = \sup_s \{-sNw - \psi_N(s)\} = -s(w)Nw - \psi_N(s(w)).$$

How does the active work (*i.e.* dissipation) control emerging behaviours?

⇒ Cloning algorithm → generate trajectories of systems of ABPs where large deviations of the active work are typical.

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→ Look for singularities in I_N/N and ψ_N/N ⇒ fundamental changes in the mechanisms to produce the associated fluctuations of the active work.

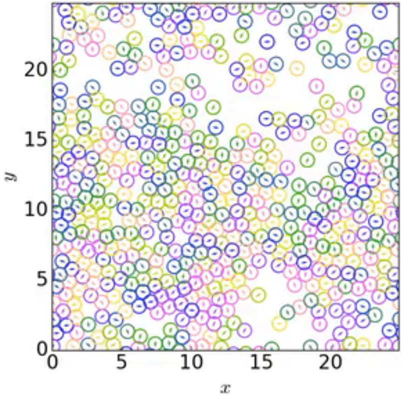


Figure: *(Movie)* Unbiased trajectory for $\phi = 0.65$, $l_p/\sigma = 40$. [from: Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605]

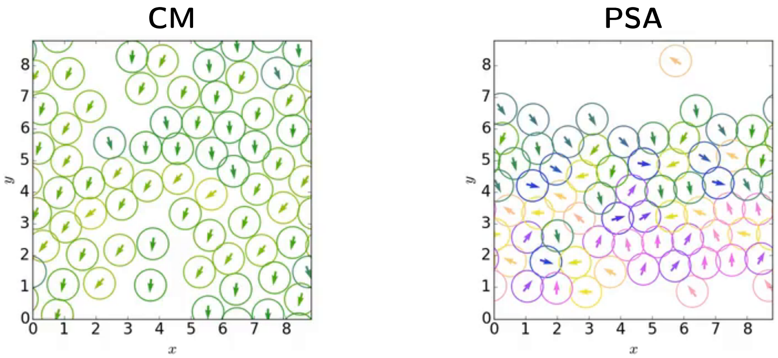


Figure: *(Movie)* Biased trajectories for $N = 64$, $\phi = 0.65$, $l_p/\sigma = 40$. **(left)** $s = -3.2$. **(right)** $s = 0.8$. [from: Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605]

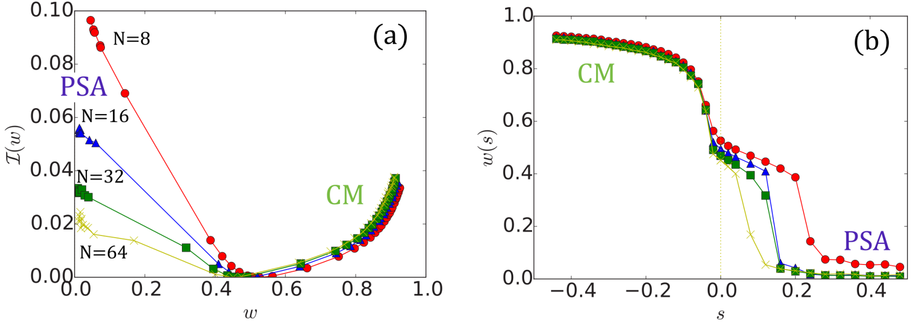


Figure: **(a)** Rescaled rate function $\mathcal{I} = I_N/N$. **(b)** Biased average of active work $w(s) = \langle w \rangle_s$. $\phi = 0.65$, $l_p/\sigma = 40$. [from: Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605]

$$\hat{\nu} = \left| \frac{1}{N} \sum_{i=1}^{N} \underline{u}_i \right| \equiv \text{global order parameter}, \;\; \nu_\tau = \frac{1}{\tau} \int_0^\tau \hat{\nu}(t)\, \mathrm{d}t$$

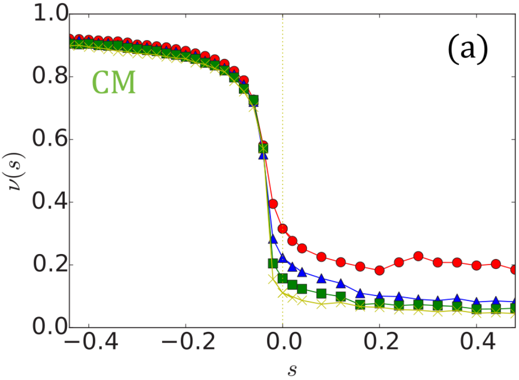
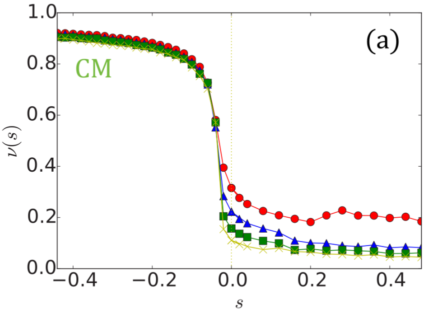


Figure: Biased average of global order parameter $\nu(s) = \langle \nu \rangle_s$. $\phi = 0.65$, $l_p/\sigma = 40$. [from: Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605]

Two limits to this study of the CM transition:

(1) Only two high persistence lengths have been considered.

(2) No claim on the locus of the CM transition.



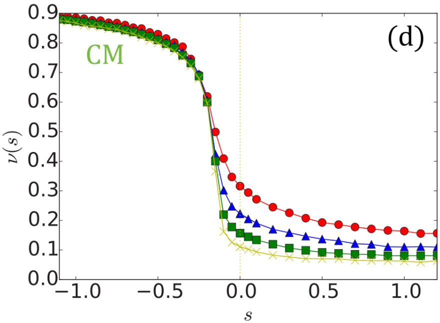
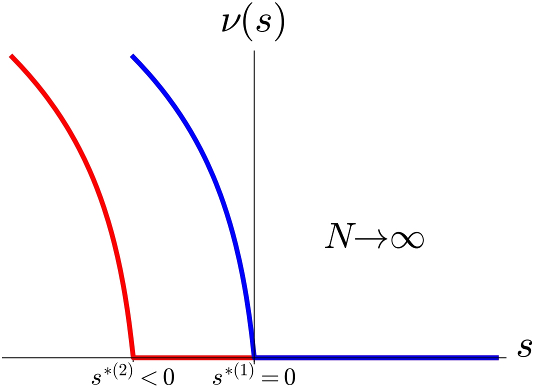


Figure: Biased average of global order parameter $\nu(s) = \langle \nu \rangle_s$. $\phi = 0.65$. **(a)** $l_p/\sigma = 40$ **(d)** $l_p/\sigma = 6.7$. [from: Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605]

→ Yet there is evidence that this locus may be affected by l_p/σ!



$\Rightarrow$ Important to disentangle active work and the coupling of orientation, and to understand the relation between them.

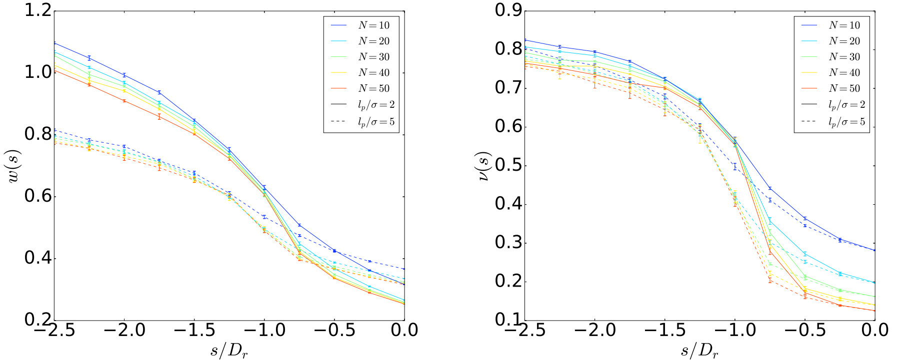


Figure: $\phi = 0.65$, $n_c = 10^2$, $t_{\text{obs}} = 10^2$. $D_r^{-1} = l_p/\sigma$. **(left)** Biased average of active work. **(right)** Biased average of the global order parameter.

$$s^* \approx -(l_p/\sigma)^{-1}$$

→ N independent Brownian rotors

$$\dot{\theta}_i = \sqrt{2D_r}\xi_i,$$

which trajectories we bias with respect to

$$\epsilon_\tau[f] = \frac{1}{\tau}\int_0^\tau f(\nu(t))\,\mathrm{d}t.$$

$\epsilon_\tau[f] \equiv$ mean energy of microstates (trajecories)

$$\epsilon_\tau^{(1)} = \frac{1}{\tau}\int_0^\tau \nu(t)\,\mathrm{d}t = \frac{1}{N\tau}\int_0^\tau \sum_{i=1}^N \cos(\theta_i(t) - \varphi(t))\,\mathrm{d}t$$

$$\approx \frac{1}{N\tau}\int_0^\tau \sum_{i=1}^N \cos(\theta_i(t))\,\mathrm{d}t$$

$\Rightarrow$ Coupling to an external field.

θ_i relax significantly faster than φ when $N \to \infty \Rightarrow \varphi$ treated as fixed external parameter.

$$\epsilon_\tau^{(1)} = \frac{1}{\tau}\int_0^\tau \nu(t)\,\mathrm{d}t = \frac{1}{N\tau}\int_0^\tau \sum_{i=1}^{N} \cos(\theta_i(t) - \varphi(t))\,\mathrm{d}t$$
$$\approx \frac{1}{N\tau}\int_0^\tau \sum_{i=1}^{N} \cos(\theta_i(t))\,\mathrm{d}t$$

$\Rightarrow$ Coupling to an external field.

$$\epsilon_\tau^{(2)} = \frac{1}{\tau}\int_0^\tau \nu^2(t)\,\mathrm{d}t = \frac{1}{N^2\tau}\int_0^\tau \sum_{i,j=1}^{N} \cos(\theta_i(t) - \theta_j(t))\,\mathrm{d}t$$

$\Rightarrow$ Coupling between each couples of rotors.

θ_i relax significantly faster than φ when $N \to \infty \Rightarrow \varphi$ treated as fixed external parameter.

$$\frac{\partial}{\partial t}P[\{\theta_i\}] = D_r \sum_{i=1}^{N} \frac{\partial^2}{\partial \theta_i^2} P[\{\theta_i\}] = \mathcal{L}P[\{\theta_i\}] \equiv \text{Fokker-Planck equation}$$

$$N\psi_{N,f}(s) = \lim_{t\to\infty} \frac{1}{\tau} \log \left\langle e^{-sN\tau\epsilon_\tau[f]} \right\rangle$$

$$\mathscr{W}_{s,f} = \mathcal{L} - sNf(\nu) \equiv \text{tilted generator},\ \mathscr{W}_{s,f}P[\{\theta_i\}] = N\psi_{N,f}(s)P[\{\theta_i\}]$$

$$\psi_{N,f}(s) = \frac{1}{N} \sup_P \frac{\int \mathrm{d}^N\{\theta_i\}\, P[\{\theta_i\}]\mathscr{W}_{s,f}P[\{\theta_i\}]}{\int \mathrm{d}^N\{\theta_i\}\, P[\{\theta_i\}]P[\{\theta_i\}]}$$

Hugo Touchette. "Introduction to dynamical large deviations of Markov processes". In: *Physica A: Statistical Mechanics and its Applications* 504 (2018), pp. 5–19.

Robert L Jack. "Ergodicity and large deviations in physical systems with stochastic dynamics". In: *arXiv preprint arXiv:1910.09883* (2019).

$$P[\{\theta_i\}] \propto \exp\left(h(s)\sum_i \cos\theta_i\right) \equiv \text{distribution ansatz}$$

$$\psi_{N,f}(s) \geq \frac{1}{N} \sup_{h(s)\in\mathbb{R}} \frac{\int \mathrm{d}^N\{\theta_i\}\, P[\{\theta_i\}] \mathscr{W}_{s,f} P[\{\theta_i\}]}{\int \mathrm{d}^N\{\theta_i\}\, P[\{\theta_i\}] P[\{\theta_i\}]} = \sup_{h(s)\in\mathbb{R}} B_{s,f}(h(s))$$

$$\langle f(\nu)\rangle_s \approx -\frac{\partial}{\partial s} \sup_{h(s)\in\mathbb{R}} B_{s,f}(h(s)) \equiv \text{approximate order parameter}$$

Approximate polarisation from bound to the SCGF

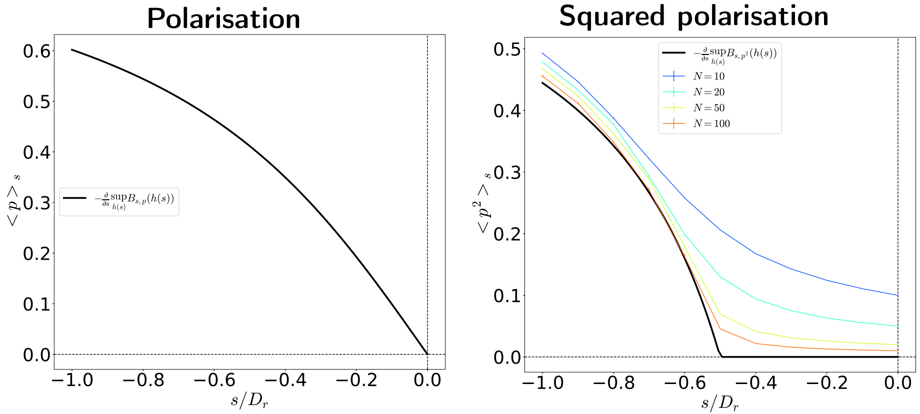


Figure: (left) Biasing with respect to polarisation. **(right)** Biasing with respect to squared polarisation. Numerical results from cloning with $n_c = 10^3$, $t_{\mathrm{obs}} = 10^2$.

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- An explicit link between active work and global polar order remains to be found.

Thank you!

Consider a sequence of random variables A_n satisfying a LDP with rate function I_A and an other sequence $B_n = h(A_n)$[1]. We then have

$$P(B_n = b) = \int_{a:h(a)=b} P(A_n = a)\,\mathrm{d}a,$$

therefore with Laplace's approximation we can write

$$P(B_n = b) \asymp \exp\left(-n \inf_{a:h(a)=b} I_A(a)\right),$$

which is equivalent to saying that B_n satisfies a LDP with a rate function

$$I_B(b) = \inf_{a:h(a)=b} I_A(a).$$

$\rightarrow$ Since probabilities are measured on the exponential scale, the probability of any large fluctuation should be approximated by the probability of the least improbable event leading to this fluctuation.

[1] h is continuous and called a contraction of A_n.

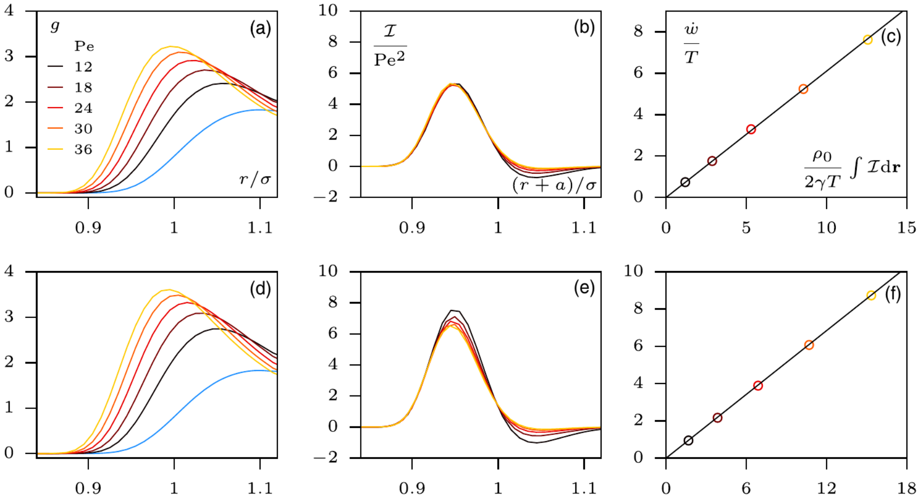

Figure: $\dot{w} \sim -w_{f,\tau}$. $\mathcal{I} = [(\nabla v)^2 - T\nabla^2 v](g - g_{eq})$. [from: Laura Tociu et al. "How Dissipation Constrains Fluctuations in Nonequilibrium Liquids: Diffusion, Structure, and Biased Interactions". In: *Physical Review X* 9.4 (2019), p. 041026]

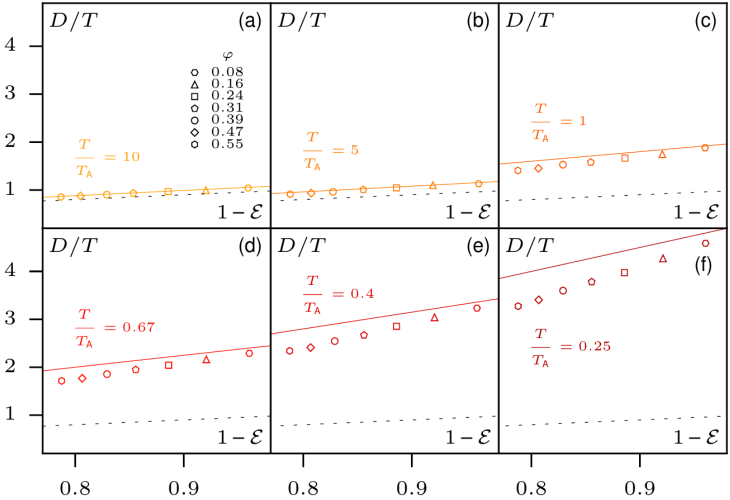

Figure: $1-\mathcal{E} \sim w$. [from: Étienne Fodor, Takahiro Nemoto, and Suriyanarayanan Vaikuntanathan. "Dissipation controls transport and phase transitions in active fluids: Mobility, diffusion and biased ensembles". In: *New Journal of Physics* (2019)]

Consider n_c copies of a system, $A^{\beta}_{N\tau,i}$ the value of observable $A_{N\tau}$ for copy i on interval $[(\beta-1)\tau, \beta\tau]$, and

$$\Upsilon_i^{\beta} = e^{sN\tau A^{\beta}_{N\tau,i}},\ \Upsilon^{\beta} = \frac{1}{n_c}\sum_{i=1}^{n_c}\Upsilon_i^{\beta},\ \omega_i^{\beta} = \frac{\Upsilon_i^{\beta}}{\Upsilon^{\beta}},$$

the associated weight factors. At each cloning time step τ, we clone each copies ω_i^{β} times, so that we get the probability of observing a given trajectory with this algorithm[2]

$$P_{\mathrm{clo}}(\{A^{\beta}_{N\tau,i}\}^{\gamma}_{\beta=1}) = P_0(\{A^{\beta}_{N\tau,i}\}^{\gamma}_{\beta=1})\frac{\prod_{\beta=1}^{\gamma}\Upsilon_i^{\beta}}{\prod_{\beta=1}^{\gamma}\Upsilon^{\beta}} = \frac{P_s(\{A^{\beta}_{N\tau,i}\}^{\gamma}_{\beta=1})}{\prod_{\beta=1}^{\gamma}\Upsilon^{\beta}},$$

then for $n_c \gg 1$

$$\prod_{\beta=1}^{\gamma}\Upsilon^{\beta} \approx \int P_s(A_{N\gamma\tau})\,\mathrm{d}A_{N\gamma\tau} \Rightarrow \psi_N(s,\gamma\tau) \approx \frac{1}{\gamma\tau}\sum_{\beta=1}^{\gamma}\log\left(\frac{1}{n_c}\sum_{i=1}^{n_c}\Upsilon_i^{\beta}\right).$$

[2] Tobias Brewer et al. "Efficient characterisation of large deviations using population dynamics". In: *Journal of Statistical Mechanics: Theory and Experiment* 2018.5 (2018), p. 053204, Thibault Lestang. "Numerical simulation and rare events algorithms for the study of extreme fluctuations of the drag force acting on an obstacle immersed in a turbulent flow". PhD thesis. 2018.

$$J(\overline{\nu}) = \lim_{\tau\to\infty} -\frac{1}{\tau} \log P\left(\int_0^\tau \nu(t)\,\mathrm{d}t = \overline{\nu}\right),$$

$$I(w) = \inf_\nu I_2(w,\nu) = I_2(w,\nu(s(w))) \geq \inf_{w'} I_2(w',\nu(s(w))) = J(\nu(s(w)))$$

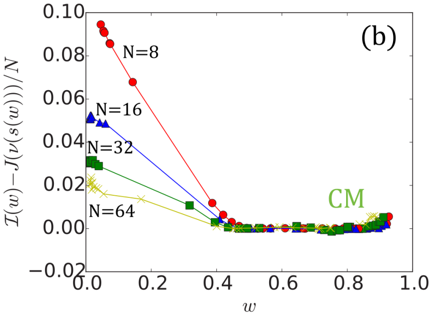

Figure: Difference of rate functions of active work and corresponding global order parameter. $\phi = 0.65$, $l_p/\sigma = 40$. We recall $\langle w \rangle_0 \approx 0.4 - 0.45$. [from: Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605]