

# Large deviations of active work in systems of active Brownian particles

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### Contents

- Active matter
  - Non-equilibrium systems
  - Active Brownian particles
- 2 Large deviation theory
  - Concepts and applications
  - Cloning algorithm
- 3 Large deviations of active work
  - PSA and CM transitions
  - Brownian rotors
- 4 Conclusion

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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).

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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.

Ludovic Berthier and Jorge Kurchan. "Lectures on non-equilibrium active systems". In: 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.
- 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.

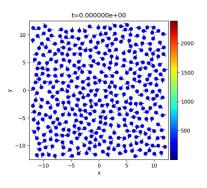
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### Non-equilibrium phenomenon in active matter: swarming

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

$$\underline{\dot{r}}_{i} = v_{0} \begin{pmatrix} \cos \theta_{i} \\ \sin \theta_{i} \end{pmatrix} - \mu \sum_{j=1}^{N} \nabla U_{ij}, \ \dot{\theta}_{i} = \frac{1}{\tau} (\varphi_{i} - \theta_{i}) + \xi_{i}, \ \varphi_{i} = \arg(\underline{\dot{r}}_{i})$$



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.

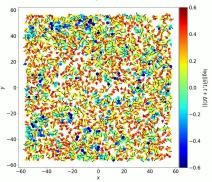
Balint Szabo et al. "Phase transition in the collective migration of tissue cells: experiment and model". In: *Physical Review E* 74.6 (2006), p. 061908.

### Non-equilibrium phenomenon in active matter: MIPS

→ Active Brownian particles with repulsive soft interactions.

$$\underline{\dot{r}}_{i} = v_{0} \begin{pmatrix} \cos \theta_{i} \\ \sin \theta_{i} \end{pmatrix} - \mu \sum_{j=1}^{N} \nabla U_{ij}, \ \dot{\theta}_{i} = \sqrt{2\tau^{-1}} \xi_{i}$$

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



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.

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

$$\begin{split} \dot{\mathcal{S}}_{N}\left[\{\underline{r}_{i},\underline{u}_{i}\}_{0}^{\tau}\right] &= \frac{1}{\tau}\log\frac{\mathcal{P}_{N}\left[\{\underline{r}_{i},\underline{u}_{i}\}_{0}^{\tau}\right]}{\mathcal{P}_{N}^{R}\left[\{\underline{r}_{i},\underline{u}_{i}\}_{0}^{\tau}\right]},\\ \dot{\mathcal{S}}_{N} &= \lim_{\tau \to \infty}\left\langle\dot{\mathcal{S}}_{N}\left[\{\underline{r}_{i},\underline{u}_{i}\}_{0}^{\tau}\right]\right\rangle, \end{split}$$

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

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

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.

# Active Brownian particles

→ N ABPs with evolution

$$\begin{split} \underline{\dot{r}}_{i} &= -\mu \sum_{j=1}^{N} \nabla U_{ij} + v_{0} \begin{pmatrix} \cos \theta_{i} \\ \sin \theta_{i} \end{pmatrix} + \sqrt{2D} \underline{\eta}_{i}, \\ \dot{\theta}_{i} &= \sqrt{2D_{r}} \xi_{i}, \end{split}$$

 $\rightarrow$   $U_{ij} \equiv$  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,  $\phi$ ,  $\sigma$ ,  $\mu$ ,  $v_0$ , 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,  $\phi$ ,  $\mu$ , D,  $D_r$ .

ightarrow 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.

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

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$$\begin{split} \underline{\dot{r}}_{i} &= -\mu \sum_{j=1}^{N} \nabla U_{ij} + \begin{pmatrix} \cos \theta_{i} \\ \sin \theta_{i} \end{pmatrix} + \sqrt{\frac{2}{3} \frac{\sigma}{I_{p}}} \underline{\eta}_{i}, \\ \dot{\theta}_{i} &= \sqrt{2 \frac{\sigma}{I_{p}}} \xi_{i}, \end{split}$$

- $\rightarrow$   $U_{ij} \equiv$  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,  $\phi$ ,  $\mu$ ,  $\frac{I_p}{\sigma} = D_r^{-1}$ .
  - ightarrow units of space and time:  $\sigma=$  1,  $\sigma/\emph{v}_0=$  1
  - $\rightarrow$  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.

# Active Brownian particles

→ N ABPs with evolution

$$\begin{split} \underline{\dot{r}}_{i} &= -\frac{1}{3} \frac{\sigma}{l_{p}} \sum_{j=1}^{N} \nabla U_{ij} + \begin{pmatrix} \cos \theta_{i} \\ \sin \theta_{i} \end{pmatrix} + \sqrt{\frac{2}{3} \frac{\sigma}{l_{p}}} \underline{\eta}_{i}, \\ \dot{\theta}_{i} &= \sqrt{2 \frac{\sigma}{l_{p}}} \xi_{i}, \end{split}$$

- $\rightarrow$   $U_{ij} \equiv$  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,  $\phi$ ,  $\frac{l_p}{\sigma} = D_r^{-1}$ .
  - ightarrow units of space and time:  $\sigma=1$ ,  $\sigma/v_0=1$
  - $\rightarrow$  Stokes-Einstein-Debye relation:  $D = \frac{1}{3}D_r$
  - $\rightarrow \mu = D$

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

$$\begin{split} \dot{\mathcal{S}}_{N} &= \lim_{\tau \to \infty} \left\langle \frac{1}{\tau} \log \frac{\mathcal{P}_{N} \left[ \left\{ \underline{r}_{i}, \underline{u}_{i} \right\}_{0}^{\tau} \right]}{\mathcal{P}_{N}^{R} \left[ \left\{ \underline{r}_{i}, \underline{u}_{i} \right\}_{0}^{\tau} \right]} \right\rangle = 3 \frac{I_{p}}{\sigma} N \lim_{\tau \to \infty} \left\langle w_{\tau} \right\rangle \\ w_{\tau} &= \frac{1}{N\tau} \int_{0}^{\tau} \sum_{i=1}^{N} \underline{\dot{r}}_{i}(t) \cdot \underline{u}(\theta_{i}(t)) \, \mathrm{d}t \\ &= \frac{1}{N\tau} \int_{0}^{\tau} \sum_{i=1}^{N} \left( 1 - \frac{1}{3} \frac{\sigma}{I_{p}} \sum_{j=1}^{N} \underline{u}(\theta_{i}) \cdot \nabla U_{ij} + \sqrt{\frac{2}{3} \frac{\sigma}{I_{p}}} \underline{u}(\theta_{i}) \cdot \underline{\eta}_{i} \right) \, \mathrm{d}t \end{split}$$

$$\dot{\mathcal{S}}_{N} = \lim_{\tau \to \infty} \left\langle \frac{1}{\tau} \log \frac{\mathcal{P}_{N}\left[ \left\{ \underline{r}_{i}, \underline{u}_{i} \right\}_{0}^{\tau} \right]}{\mathcal{P}_{N}^{R}\left[ \left\{ \underline{r}_{i}, \underline{u}_{i} \right\}_{0}^{\tau} \right]} \right\rangle = 3 \frac{I_{p}}{\sigma} N \lim_{\tau \to \infty} \left\langle w_{\tau} \right\rangle$$

$$w_{\tau} = \frac{1}{N\tau} \int_{0}^{\tau} \sum_{i=1}^{N} \underline{\dot{r}}_{i}(t) \cdot \underline{u}(\theta_{i}(t)) dt$$

$$= \frac{1}{N\tau} \int_{0}^{\tau} \sum_{i=1}^{N} \left( 1 - \frac{1}{3} \frac{\sigma}{I_{p}} \sum_{j=1}^{N} \underline{u}(\theta_{i}) \cdot \nabla U_{ij} + \sqrt{\frac{2}{3} \frac{\sigma}{I_{p}}} \underline{u}(\theta_{i}) \cdot \underline{\eta}_{i} \right) dt$$

# **Flocking**



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

# **Jamming**



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

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# Large deviation principle

 $\rightarrow X_1, \dots, X_n$  a sequence of random numbers and its sample average

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

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

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

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

# LDP example: sample mean of Gaussian random variables

 $\to X_1, \dots, X_n$  random numbers from a Gaussian distribution  $(\mu, \sigma)$ .

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

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

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

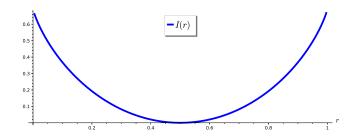
 $\Rightarrow$   $S_n$  satisfies a large deviation principle.

# LDP example: mean of random bits

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

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

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

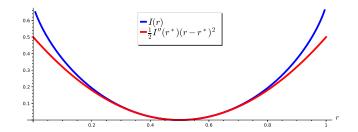


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ightarrow Deviations from the Gaussian fluctuations predicted by the Central Limit Theorem  $\Rightarrow$  *large* deviations.

Scaled cumulant generating function (SCGF)

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

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

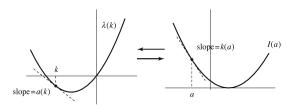


Figure: [from: Hugo Touchette. "The large deviation approach to statistical mechanics". In: *Physics Reports* 478.1-3 (2009), pp. 1–69]

# Analogy with equilibrium statistical mechanics: free energy

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

$$\psi(\Delta\beta) = \lim_{n \to \infty} \frac{1}{n} \log \int e^{\Delta\beta n E_n(\omega)} P_{\beta}(\omega) d\omega = \lim_{n \to \infty} \frac{1}{n} \log \frac{Z_n(\beta - \Delta\beta)}{Z_n(\beta)}$$
$$= \beta F(\beta) - (\beta - \Delta\beta) F(\beta - \Delta\beta)$$
$$F(\beta) = -\frac{1}{\beta} \lim_{n \to \infty} \frac{1}{n} \log Z_n(\beta) \equiv \text{free energy density}$$

# Analogy with equilibrium statistical mechanics: entropy

$$\psi$$
 is differentiable  $\Longrightarrow$   $P_{\beta}(E_n) \simeq \exp(-nI_{\beta}(E_n))$ 

$$P_{eta}(E_n)symp \exp(n(\underbrace{s(E_n)}_{ ext{entropy}}-\widehat{eta}E_n+\underbrace{eta F(eta)}_{ ext{partition}}))$$
 $= \text{number of states}$ 
 $I_{eta}(E_n)=-s(E_n)-eta E_n+eta F(eta)$ 
 $I_{eta}(E_n)=0\Leftrightarrow F(eta)=E_n-rac{1}{eta}s(E_n)$ 

# Application to trajectories: dynamical phase transitions

 $\rightarrow$  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 <sub>i</sub>	Microstates of $(d+1)$ -dimensional system
$A_{N au}$	Mean energy
S	Inverse temperature (conjugate to the energy)
$\psi_{ extsf{N}}$	Free energy difference
$I_N$	$-s(E_n) - \beta E_n + \beta F(\beta)$

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

# Cloning algorithm

$$Z_{ au}(s) = \left\langle e^{sN_{ au}A_{N_{ au}}} 
ight
angle \equiv rac{dynamical}{ ext{of a Boltzmann-like measure}}$$

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

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- $\rightarrow s \neq 0 \Rightarrow$  average dominated by trajectories with rare events.
- ⇒ Cloning algorithm to generate the biased measure.

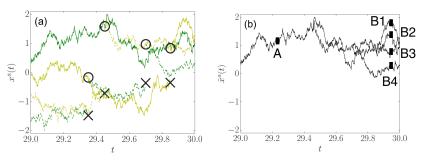


Figure:  $Z_{\tau}(s) = \left\langle \exp\left(s \int_0^{\tau} x(t)(1+x(t)) \, \mathrm{d}t\right) \right\rangle$ . [from: Takahiro Nemoto et al. "Population-dynamics method with a multicanonical feedback control". In: *Physical Review E* 93.6 (2016), p. 062123]

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### Method

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...

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

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

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

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

... and rate function.

$$I_N(w) = \sup_{s} \left\{ -sNw - \psi_N(s) \right\} = -s(w)Nw - \psi_N(s(w)).$$

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

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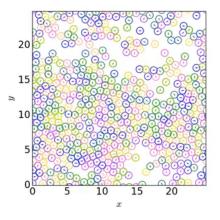
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 $\rightarrow$  Look for singularities in  $I_N/N$  and  $\psi_N/N \Rightarrow$  fundamental changes in the mechanisms to produce the associated fluctuations of the active work.



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

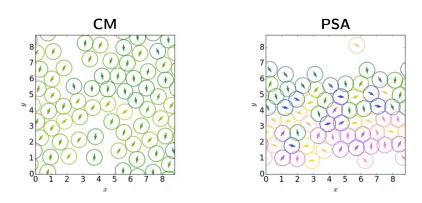
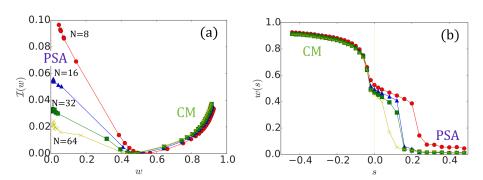


Figure: (Movie) Biased trajectories for N=64,  $\phi=0.65$ ,  $I_p/\sigma=40$ . (left) s=-3.2. (right) s=0.8. [from: Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605]



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

## Analysis of the CM transition

$$\hat{\nu} = \left| \frac{1}{N} \sum_{i=1}^{N} \underline{u}_i \right| \equiv ext{global order parameter}, \ 
u_{ au} = \frac{1}{ au} \int_{0}^{ au} \hat{
u}(t) \, \mathrm{d}t$$

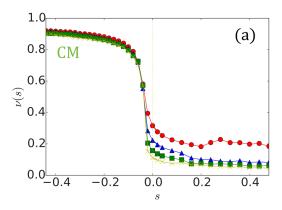


Figure: Biased average of global order parameter  $\nu(s) = \langle \nu \rangle_s$ .  $\phi = 0.65$ ,  $I_p/\sigma = 40$ . [from: Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605]

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.

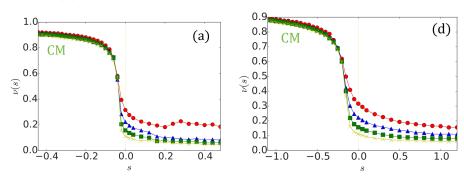
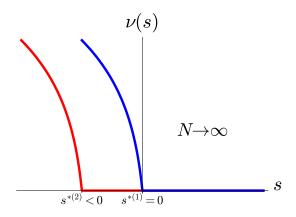


Figure: Biased average of global order parameter  $\nu(s)=\langle \nu \rangle_s$ .  $\phi=0.65$ . (a)  $I_p/\sigma=40$  (d)  $I_p/\sigma=6.7$ . [from: Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p.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

 $\rightarrow$  Yet there is evidence that this locus may be affected by  $I_p/\sigma!$ 

## Significance of the locus of the CM transition



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

### Evidence for a CM transition at finite $s^*$

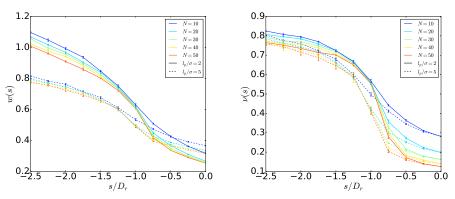


Figure:  $\phi=0.65$ ,  $n_c=10^2$ ,  $t_{\rm obs}=10^2$ .  $D_r^{-1}=l_p/\sigma$ . (left) Biased average of active work. (right) Biased average of the global order parameter.

$$s^* pprox - (I_p/\sigma)^{-1}$$

## Independent Brownian rotors

→ N independent Brownian rotors

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

which trajectories we bias with respect to

$$\epsilon_{ au}[f] = rac{1}{ au} \int_0^{ au} f(
u(t)) \, \mathrm{d}t.$$

 $\epsilon_{ au}[f] \equiv$  mean energy of microstates (trajecories)

#### Choice of the bias

$$egin{aligned} \epsilon_{ au}^{(1)} &= rac{1}{ au} \int_0^ au 
u(t) \, \mathrm{d}t = rac{1}{N au} \int_0^ au \sum_{i=1}^N \cos( heta_i(t) - arphi(t)) \, \mathrm{d}t \ &pprox rac{1}{N au} \int_0^ au \sum_{i=1}^N \cos( heta_i(t)) \, \mathrm{d}t \end{aligned}$$

⇒ Coupling to an external field.

 $<sup>\</sup>theta_i$  relax significantly faster than  $\varphi$  when  $N \to \infty \Rightarrow \varphi$  treated as fixed external parameter.

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$$\epsilon_{ au}^{(2)} = rac{1}{ au} \int_{0}^{ au} 
u^{2}(t) dt = rac{1}{N^{2} au} \int_{0}^{ au} \sum_{i,i=1}^{N} \cos(\theta_{i}(t) - \theta_{j}(t)) dt$$

⇒ Coupling between each couples of rotors.

 $<sup>\</sup>theta_i$  relax significantly faster than  $\varphi$  when  $N \to \infty \Rightarrow \varphi$  treated as fixed external parameter.

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

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

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

$$\psi_{N,f}(s) = \frac{1}{N} \sup_{P} \frac{\int d^{N}\{\theta_{i}\} P[\{\theta_{i}\}] \mathscr{W}_{s,f} P[\{\theta_{i}\}]}{\int d^{N}\{\theta_{i}\} P[\{\theta_{i}\}] P[\{\theta_{i}\}]}$$

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

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

## Ansatz for the joint distribution of orientations

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

$$\psi_{N,f}(s) \geq \frac{1}{N} \sup_{h(s) \in \mathbb{R}} \frac{\int \mathsf{d}^N \{\theta_i\} \, P[\{\theta_i\}] \mathscr{W}_{s,f} P[\{\theta_i\}]}{\int \mathsf{d}^N \{\theta_i\} \, P[\{\theta_i\}] P[\{\theta_i\}]} = \sup_{h(s) \in \mathbb{R}} B_{s,f}(h(s))$$
$$\langle f(\nu) \rangle_s \approx -\frac{\partial}{\partial s} \sup_{h(s) \in \mathbb{R}} B_{s,f}(h(s)) \equiv \text{approximate order parameter}$$

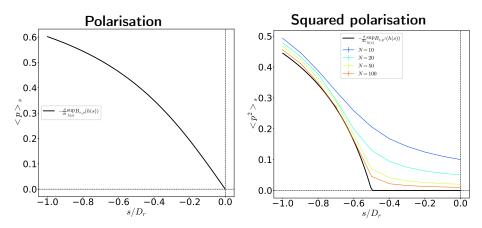


Figure: (left) Biasing with respect to polarisation. (right) Biasing with respect to squared polarisation. Numerical results from cloning with  $n_c = 10^3$ ,  $t_{\rm obs} = 10^2$ .

#### Contents

- Active matter
  - Non-equilibrium systems
  - Active Brownian particles
- 2 Large deviation theory
  - Concepts and applications
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- 3 Large deviations of active work
  - PSA and CM transitions
  - Brownian rotors
- 4 Conclusion

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

# Thank you!

## Contraction principle

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

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

therefore with Laplace's approximation we can write

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

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

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

→ 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.

<sup>&</sup>lt;sup>1</sup> h is continuous and called a contraction of  $A_n$ .

## Dissipation and structure

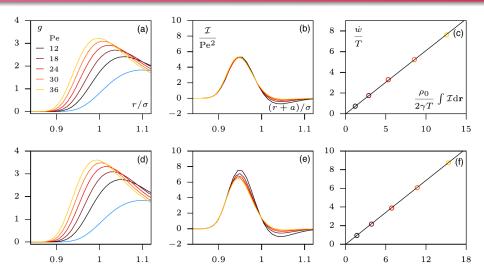


Figure:  $\dot{w} \sim -w_{f,\tau}$ .  $\mathcal{I} = [(\nabla v)^2 - T\nabla^2 v](g - g_{eq})$ . [from: Laura Tociu et al. "How Dissipation Constrains Fluctuations in Nonequilibrium Liquids: Diffusion, Structure, and Biased Interactions". In: *Physical Review X* 9.4 (2019), p. 041026]

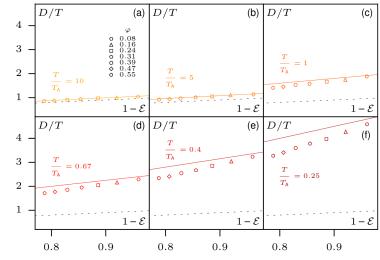


Figure:  $1-\mathcal{E} \sim w$ . [from: Étienne Fodor, Takahiro Nemoto, and Suriyanarayanan Vaikuntanathan. "Dissipation controls transport and phase transitions in active fluids: Mobility, diffusion and biased ensembles". In: New Journal of Physics (2019)]

## Cloning algorithm

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

$$\Upsilon_{i}^{\beta} = e^{sN\tau A_{N\tau,i}^{\beta}}, \ \Upsilon^{\beta} = \frac{1}{n_{c}} \sum_{i=1}^{n_{c}} \Upsilon_{i}^{\beta}, \ \omega_{i}^{\beta} = \frac{\Upsilon_{i}^{\beta}}{\Upsilon^{\beta}},$$

the associated weight factors. At each cloning time step  $\tau$ , we clone each copies  $\omega_i^\beta$  times, so that we get the probability of observing a given trajectory with this algorithm<sup>2</sup>

$$P_{\mathsf{clo}}(\{A_{N\tau,i}^{\beta}\}_{\beta=1}^{\gamma}) = P_{\mathsf{0}}(\{A_{N\tau,i}^{\beta}\}_{\beta=1}^{\gamma}) \frac{\prod_{\beta=1}^{\gamma} \Upsilon_{i}^{\beta}}{\prod_{\beta=1}^{\gamma} \Upsilon^{\beta}} = \frac{P_{\mathsf{s}}(\{A_{N\tau,i}^{\beta}\}_{\beta=1}^{\gamma})}{\prod_{\beta=1}^{\gamma} \Upsilon^{\beta}},$$

then for  $n_c\gg 1$ 

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

<sup>&</sup>lt;sup>2</sup>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.

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

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

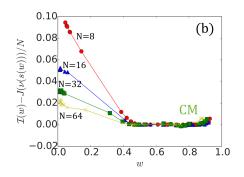


Figure: Difference of rate functions of active work and corresponding global order parameter.  $\phi = 0.65$ ,  $I_p/\sigma = 40$ . We recall  $\langle w \rangle_0 \approx 0.4 - 0.45$ . [from: Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming".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