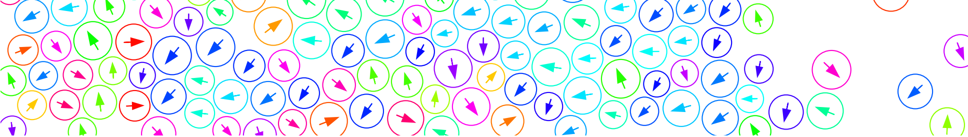


Collective motion in large deviations of active particles

Yann-Edwin Keta

supervised by Robert Jack and Frédéric van Wijland

21/09/2020

arXiv:2009.07112

yketa/DAMTP_MSC_2019_Wiki

1. Model and methods
   - Active Brownian particles
   - Large deviations of active work
2. 2 RTPs on a ring
3. Large deviations of ABPs
   - Polarisation
   - Transition to collective motion
   - Passive limit

1 Model and methods
- Active Brownian particles
- Large deviations of active work

2 2 RTPs on a ring

3 Large deviations of ABPs
- Polarisation
- Transition to collective motion
- Passive limit

ABP

$$\dot{\boldsymbol{r}}_i = v_0 \begin{pmatrix} \cos\theta_i \\ \sin\theta_i \end{pmatrix} - \mu \nabla_i U + \sqrt{2D}\boldsymbol{\eta}_i$$

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

$$\left\langle \eta_i^\alpha(t)\eta_j^\beta(t') \right\rangle = \delta_{\alpha\beta}\delta_{ij}\delta(t-t')$$

$$\left\langle \xi_i(t)\xi_j(t') \right\rangle = \delta_{ij}\delta(t-t')$$

$$\left\langle \boldsymbol{u}(\theta_i(t)) \cdot \boldsymbol{u}(\theta_j(t')) \right\rangle = \delta_{ij} e^{-D_r|t-t'|}$$

WCA

$$U = \varepsilon \sum_{1\leq i<j\leq N} \left[4\left((r_{ij}/\sigma)^{-12} - (r_{ij}/\sigma)^{-6}\right) + 1\right] \Theta(2^{1/6} - r_{ij}/\sigma)$$

- length: $\sigma = 1$, energy: $\varepsilon = 1$, time: $\sigma/v_0 = 1$
- $\mu = D/\varepsilon$, $D_r = 3D/\sigma^2$
- $\phi = N\pi\sigma^2/(4L^2) = 0.65$, $\tilde{l}_{\mathrm{p}} = v_0/(\sigma D_r)$

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

instantaneous dissipated power: $\dot{\mathcal{W}} = \sum_i \dot{\boldsymbol{r}}_i \circ \frac{1}{D}\left(\dot{\boldsymbol{r}}_i - \sqrt{2D}\boldsymbol{\eta}_i\right)$

instantaneous dissipated power: $\dot{\mathcal{W}} = \sum_i \dot{\boldsymbol{r}}_i \circ \frac{1}{D}\left(\dot{\boldsymbol{r}}_i - \sqrt{2D}\boldsymbol{\eta}_i\right)$

$$\frac{1}{\tau}\int_0^\tau \dot{\mathcal{W}}(t)\,\mathrm{d}t = \frac{Nv_0^2}{D} w_\tau + \frac{1}{\tau}[U(\tau) - U(0)]$$

$$w_\tau = \frac{1}{v_0 N\tau}\sum_{i=1}^N \int_0^\tau \boldsymbol{u}(\theta_i)\circ \mathrm{d}\boldsymbol{r}_i \qquad \textbf{(active work)}$$

$$= 1 + \underbrace{\frac{-D}{v_0 N\tau}\sum_{i=1}^N \int_0^\tau \boldsymbol{u}(\theta_i)\circ \nabla_i U\,\mathrm{d}t}_{w_{f,\tau}} + \underbrace{\frac{1}{v_0 N\tau}\sum_{i=1}^N \int_0^\tau \boldsymbol{u}(\theta_i)\circ \sqrt{2D}\boldsymbol{\eta}_i\,\mathrm{d}t}_{w_{\eta,\tau}}$$

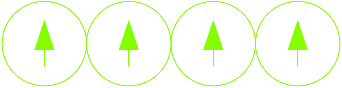
instantaneous dissipated power: $\dot{\mathcal{W}} = \sum_i \dot{\boldsymbol{r}}_i \circ \frac{1}{D}\left(\dot{\boldsymbol{r}}_i - \sqrt{2D}\boldsymbol{\eta}_i\right)$

$$\frac{1}{\tau}\int_0^\tau \dot{\mathcal{W}}(t)\,\mathrm{d}t = \frac{Nv_0^2}{D} w_\tau + \frac{1}{\tau}[U(\tau) - U(0)]$$

$$w_\tau = \frac{1}{v_0 N\tau}\sum_{i=1}^N \int_0^\tau \boldsymbol{u}(\theta_i)\circ \mathrm{d}\boldsymbol{r}_i \qquad \textbf{(active work)}$$

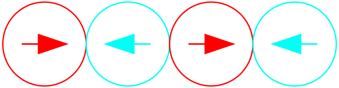
$$= 1 + \underbrace{\frac{-D}{v_0 N\tau}\sum_{i=1}^N \int_0^\tau \boldsymbol{u}(\theta_i)\circ \nabla_i U\,\mathrm{d}t}_{w_{f,\tau}} + \underbrace{\frac{1}{v_0 N\tau}\sum_{i=1}^N \int_0^\tau \boldsymbol{u}(\theta_i)\circ \sqrt{2D}\boldsymbol{\eta}_i\,\mathrm{d}t}_{w_{\eta,\tau}}$$

Flocking



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

Jamming



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

$$\textbf{biased average: } \langle \mathcal{A} \rangle_s = \frac{\left\langle \mathcal{A} e^{-sN\tau w_\tau} \right\rangle}{\left\langle e^{-sN\tau w_\tau} \right\rangle}$$

$$\textbf{biased average:}\ \langle\mathcal{A}\rangle_s = \frac{\left\langle \mathcal{A} e^{-sN\tau w_\tau} \right\rangle}{\left\langle e^{-sN\tau w_\tau} \right\rangle} = \frac{\left\langle \mathcal{A} e^{-sN\tau w_{f,\tau}} \right\rangle_{v_s^{\mathrm{con}}}}{\left\langle e^{-sN\tau w_{f,\tau}} \right\rangle_{v_s^{\mathrm{con}}}}$$

$$v_s^{\mathrm{con}} = v_0 \left(1 - \frac{2sD}{v_0^2}\right)$$

biased average: $\langle \mathcal{A} \rangle_s = \frac{\left\langle \mathcal{A} e^{-sN\tau w_\tau} \right\rangle}{\left\langle e^{-sN\tau w_\tau} \right\rangle} = \frac{\left\langle \mathcal{A} e^{-sN\tau w_{f,\tau}} \right\rangle_{v_s^{\mathrm{con}}}}{\left\langle e^{-sN\tau w_{f,\tau}} \right\rangle_{v_s^{\mathrm{con}}}}$

$$v_s^{\mathrm{con}} = v_0 \left(1 - \frac{2sD}{v_0^2} \right)$$

$$w^{\mathrm{free}}(s) = \langle w_\tau \rangle_{s,U=0} = 1 - \frac{2sD}{v_0^2}$$

$$s^{\mathrm{con}} = s \left(1 - \frac{2sD}{v_0^2} \right), \; s w_{f,\tau} = s^{\mathrm{con}} \frac{w_{f,\tau}}{w_{free}(s)}$$

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

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

$\Rightarrow$ *Cloning algorithm*: simulate $n_c \gg 1$ copies of the system and clones/deletes them at regular intervals to enforce biased measure.

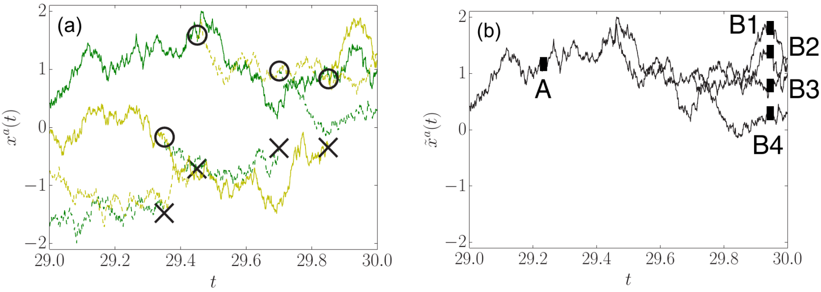


Figure: $Z_\tau(s) = \left\langle \exp\left(s \int_0^\tau x(t)(1 + x(t))\,\mathrm{d}t\right)\right\rangle$, $s = 1$. [from: Takahiro Nemoto et al. "Population-dynamics method with a multicanonical feedback control". In: *Physical Review E* 93.6 (2016), p. 062123]

1. Model and methods
   - Active Brownian particles
   - Large deviations of active work
2. 2 RTPs on a ring
3. Large deviations of ABPs
   - Polarisation
   - Transition to collective motion
   - Passive limit

RTP

$$\dot{r}_i = \alpha_i v_0 - \frac{\partial}{\partial r_i} V(r_{12})$$

tumble $(\alpha_i \to -\alpha_i)$ rate: τ_{p}^{-1}

ring length: L, persistence length: $l = v_0 \tau_{\mathrm{p}}$

potential

$$\lim_{r_{12}\to 0} V(r_{12}) = \infty$$

$$V(r_{12} > \varepsilon) = 0$$

$$\frac{\partial}{\partial r_1} V(r_{12} = r^*) = -v_0$$

hard core limit:

$\varepsilon \to 0,\ r^* \to 0$

active work

$$\dot{w}_f^{\mathrm{RTP}} = v_0(\alpha_1 - \alpha_2)\frac{\partial}{\partial r_1} V(r_{12}) = \begin{cases} -2v_0^2 & \text{if contact} \\ 0 & \text{otherwise} \end{cases}$$

$$\langle \mathcal{A} \rangle_\lambda = \frac{\left\langle \mathcal{A} e^{-\lambda \int_0^\tau \dot{w}_f^{\mathrm{RTP}}(t)\,\mathrm{d}t} \right\rangle}{\left\langle e^{-\lambda \int_0^\tau \dot{w}_f^{\mathrm{RTP}}(t)\,\mathrm{d}t} \right\rangle}$$

polarisation

$$\nu^{\mathrm{RTP}} = \frac{1 + \alpha_1 \alpha_2}{2}$$

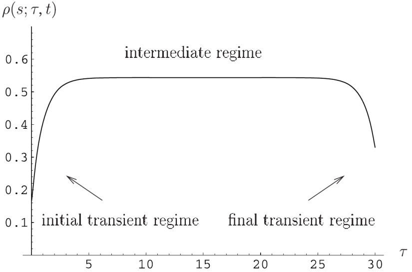


Figure: Example trajectory for the λ-ensemble (s-ensembe) of trajectories of length $t = 30$. [from: Juan P Garrahan et al. "First-order dynamical phase transition in models of glasses: an approach based on ensembles of histories". In: *Journal of Physics A: Mathematical and Theoretical* 42.7 (2009), p. 075007]

intermediate regime

$$\nu_{\mathrm{ave}}^{\mathrm{RTP}}(\lambda) = \lim_{\tau\to\infty} \left\langle \frac{1}{\tau} \int_0^{\tau} \nu^{\mathrm{RTP}}(t)\,\mathrm{d}t \right\rangle_{\lambda}$$

final regime

$$\nu_{\mathrm{end}}^{\mathrm{RTP}}(\lambda) = \left\langle \nu^{\mathrm{RTP}} \right\rangle_{\lambda}$$

dynamical free energy density: $\psi^{\mathrm{RTP}}(\lambda) = \lim_{\tau\to\infty} \frac{1}{\tau} \log \left\langle \exp\left(-\lambda \int_0^\tau \dot{w}_f^{\mathrm{RTP}}(t)\,\mathrm{d}t\right)\right\rangle$

$$\psi^{\mathrm{RTP}}(\lambda)\boldsymbol{P}_\lambda = \left(\boldsymbol{\mathcal{L}} - \lambda \dot{w}_f^{\mathrm{RTP}}\boldsymbol{I}\right)\boldsymbol{P}_\lambda \qquad \psi^{\mathrm{RTP}}(\lambda)\boldsymbol{Q}_\lambda = \left(\boldsymbol{\mathcal{L}}^\dagger - \lambda \dot{w}_f^{\mathrm{RTP}}\boldsymbol{I}\right)\boldsymbol{Q}_\lambda$$

$\boldsymbol{\mathcal{L}}, \boldsymbol{\mathcal{L}}^\dagger \equiv$ forward and backward Fokker-Planck operators

$$\begin{aligned}
\boldsymbol{P}_\lambda^{\mathrm{end}} &\equiv P_\lambda^{\alpha_1\alpha_2}(r) \\
&= \varepsilon_\lambda^{\alpha_1\alpha_2}(r) + \gamma_\lambda^{\alpha_1\alpha_2,\mathrm{l}}\delta(r) + \gamma_\lambda^{\alpha_1\alpha_2,\mathrm{r}}\delta(L-r) \\
\nu_{\mathrm{end}}^{\mathrm{RTP}}(\lambda) &= \int_0^L \left(P_\lambda^{++}(r) + P_\lambda^{--}(r)\right)\mathrm{d}r
\end{aligned}$$

$$\begin{aligned}
\boldsymbol{P}_\lambda^{\mathrm{ave}} &\equiv \hat{P}_\lambda^{\alpha_1\alpha_2}(r) = P_\lambda^{\alpha_1\alpha_2}(r)Q_\lambda^{\alpha_1\alpha_2}(r) \\
&= \hat{\varepsilon}_\lambda^{\alpha_1\alpha_2}(r) + \hat{\gamma}_\lambda^{\alpha_1\alpha_2,\mathrm{l}}\delta(r) + \hat{\gamma}_\lambda^{\alpha_1\alpha_2,\mathrm{r}}\delta(L-r) \\
\nu_{\mathrm{ave}}^{\mathrm{RTP}}(\lambda) &= \int_0^L \left(\hat{P}_\lambda^{++}(r) + \hat{P}_\lambda^{--}(r)\right)\mathrm{d}r
\end{aligned}$$

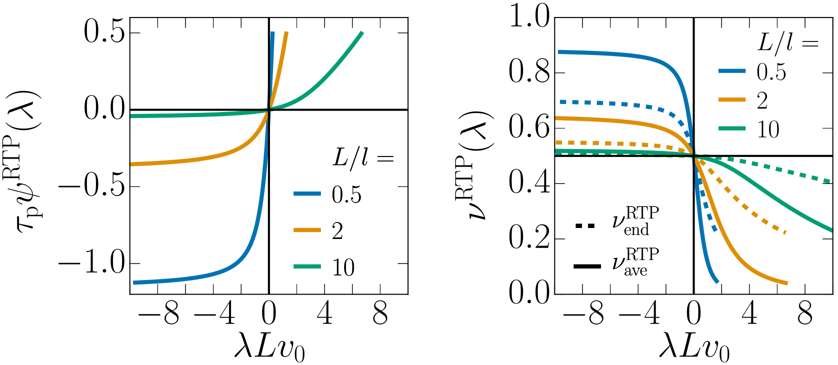


Figure: **(left)** Dynamical free energy density. **(right)** Polarisation. [from: Yann-Edwin Keta et al. "Collective motion in large deviations of active particles". In: *arXiv preprint arXiv:2009.07112* (2020)]

$$-\frac{\partial}{\partial\lambda}\psi^{\mathrm{RTP}}(\lambda) = \left\langle w_f^{\mathrm{RTP}} \right\rangle_\lambda$$

1. Model and methods
   - Active Brownian particles
   - Large deviations of active work
2. 2 RTPs on a ring
3. Large deviations of ABPs
   - Polarisation
   - Transition to collective motion
   - Passive limit

polarisation: $\hat{\nu} = \left| \frac{1}{N} \sum_{i=1}^{N} \boldsymbol{u}(\theta_i) \right|, \ \bar{\nu}_\tau = \frac{1}{\tau} \int_0^\tau \hat{\nu}(t)\, \mathrm{d}t, \ \hat{\nu} e^{\mathrm{i}\varphi} = \frac{1}{N} \sum_{i=1}^{N} e^{\mathrm{i}\theta_i}$

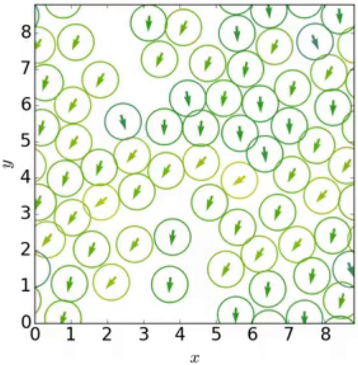


Figure: *(Movie)* Biased trajectory for $N = 64$, $\phi = 0.65$, $\tilde{l}_{\mathrm{p}} = 40$, $s = -3.2$. [from: Takahiro Nemoto et al. "Optimizing active work: Dynamical phase transitions, collective motion, and jamming". In: *Physical Review E* 99.2 (2019), p. 022605]

modified swim speed: $\dot{\boldsymbol{r}}_i = v_s^{\mathrm{con}} \boldsymbol{u}(\theta_i) - D\nabla_i U + \sqrt{2D}\boldsymbol{\eta}_i$

aligning torque: $\dot{\theta}_i = -D_r \dfrac{\partial}{\partial \theta_i}\left(-\dfrac{gN}{D_r}|\boldsymbol{\nu}|^2\right) + \sqrt{2D_r}\xi_i$

$$P[\{\boldsymbol{r}_i, \theta_i\}] \exp(-sN\tau w_\tau) \propto P^{\mathrm{mod}}[\{\boldsymbol{r}_i, \theta_i\}] \exp(-sN\tau w_\tau^{\mathrm{mod}})$$

$$s w_\tau^{\mathrm{mod}} = s\left(1 - \frac{sD}{v_0^2} + w_{f,\tau}\right) - g\left(\frac{1}{N} - \mathcal{I}_{1,\tau} + \frac{g}{D_r}\mathcal{I}_{2,\tau}\right)$$

$$\mathcal{I}_{1,\tau} = \frac{1}{\tau}\int_0^\tau |\boldsymbol{\nu}(t)|^2 \,\mathrm{d}t$$

$$\mathcal{I}_{2,\tau} = \frac{1}{N\tau}\int_0^\tau |\boldsymbol{\nu}(t)|^2 \sum_{i=1}^{N} \sin(\theta_i(t) - \varphi(t))^2 \,\mathrm{d}t$$

dynamical free energy density: $\psi(s) = \lim_{\tau \to \infty} \frac{1}{N\tau} \log \langle \exp(-sN\tau w_\tau) \rangle$

rate function: $I(w_\tau) = -\lim_{\tau \to \infty} \frac{1}{N\tau} \log P(w_\tau) = -ws(w) - \psi(s(w))$

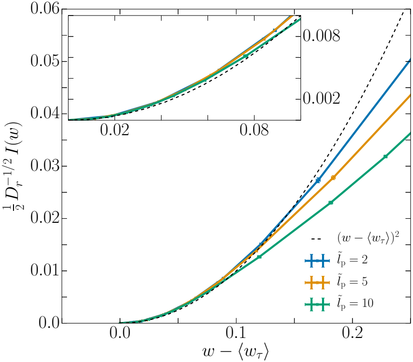


Figure: Rate function $I(w)$, $N = 50$, $\phi = 0.65$, $n_c = 10^3$, $t_{\max} = 10^3$. [from: Yann-Edwin Keta et al. "Collective motion in large deviations of active particles". In: *arXiv preprint arXiv:2009.07112* (2020)]

$\Rightarrow \ \mathrm{Var}(w_\tau) \propto D_r^{-1/2}$

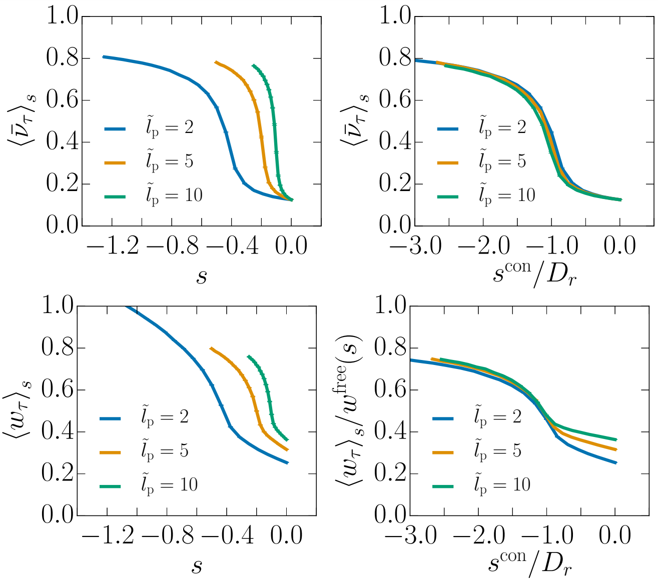


Figure: Biased averages of the polarisation $\langle \bar{\nu}_\tau \rangle_s$ and active work $\langle w_\tau \rangle_s$, $N = 50$. [from: Yann-Edwin Keta et al. "Collective motion in large deviations of active particles". In: *arXiv preprint arXiv:2009.07112* (2020)]

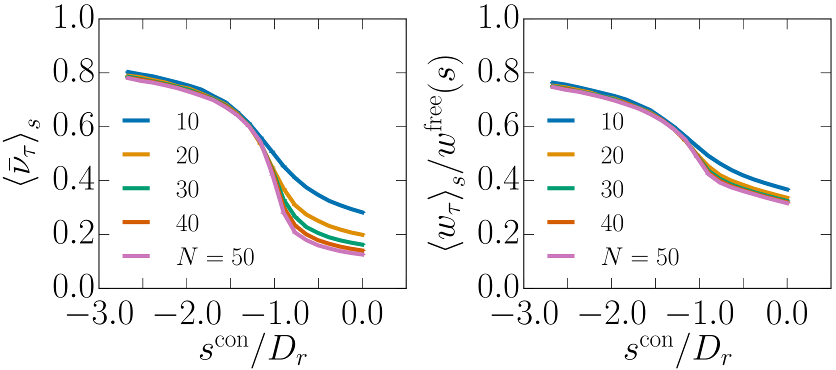


Figure: Biased averages of the polarisation $\langle \bar{\nu}_\tau \rangle_s$ and active work $\langle w_\tau \rangle_s$, $\tilde{l}_{\mathrm{p}} = 5$. [from: Yann-Edwin Keta et al. "Collective motion in large deviations of active particles". In: *arXiv preprint arXiv:2009.07112* (2020)]

$\Rightarrow$ dynamical phase transition at $s^{\mathrm{con}*} \sim -D_r$

modified swim speed: $\dot{\boldsymbol{r}}_i = v_s^{\mathrm{con}} \boldsymbol{u}(\theta_i) - D\nabla_i U + \sqrt{2D}\boldsymbol{\eta}_i$

aligning torque: $\dot{\theta}_i = -D_r \frac{\partial}{\partial \theta_i}\left(-\frac{gN}{D_r}|\boldsymbol{\nu}|^2\right) + \sqrt{2D_r}\xi_i$

$$I(w) \leq \lim_{\tau\to\infty} \frac{1}{N\tau}\mathcal{D}_{\mathrm{KL}}(P^{\mathrm{mod}}_{g(w)}||P)$$

$$\mathcal{D}_{\mathrm{KL}}(P^{\mathrm{mod}}_{g(w)}||P) = \left\langle \log \frac{P^{\mathrm{mod}}_{g(w)}}{P} \right\rangle_{\mathrm{mod}}$$

$$\lim_{\tau\to\infty} \frac{1}{N\tau}\mathcal{D}_{\mathrm{KL}}(P^{\mathrm{mod}}_{g(w)}||P) = \left\langle g(w)\mathcal{I}_{1,\tau} - \frac{g(w)^2}{D_r}\mathcal{I}_{2,\tau} \right\rangle_{\mathrm{mod}} - \frac{g(w)}{N}$$

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

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

Bounds to the rate function

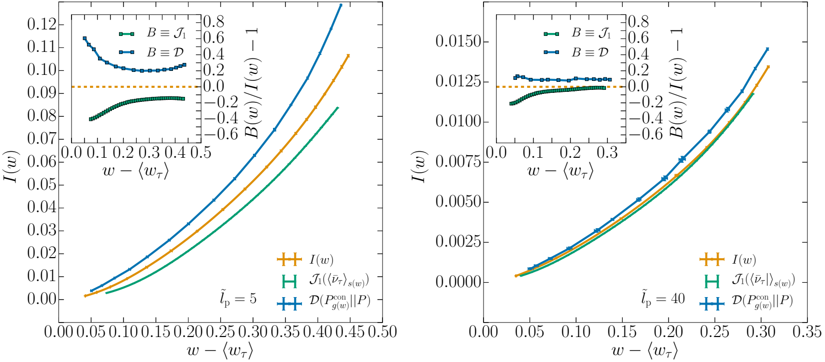


Figure: Bounds to the rate function $I(w)$. [from: Yann-Edwin Keta et al. "Collective motion in large deviations of active particles". In: *arXiv preprint arXiv:2009.07112* (2020)]

- $w > w^*$ **(CM):** fluctuations of w_τ strongly coupled to those of $\bar{\nu}_\tau$
- $w < w^*$ **(isotropic):** w_τ is enhanced by other mechanisms than orientation coupling

$$S_s(\boldsymbol{q}) = \langle \rho_{\boldsymbol{q}} \rho_{-\boldsymbol{q}} \rangle_s$$

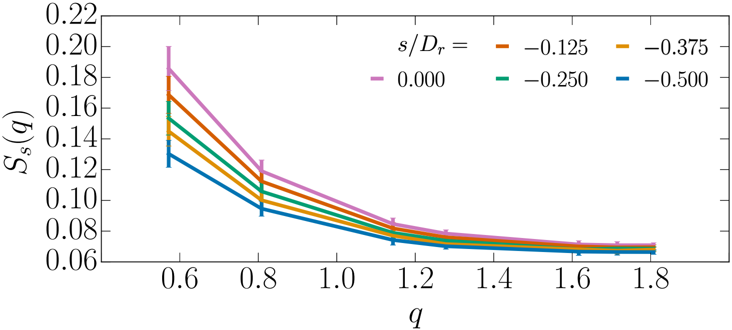


Figure: Biased structure factor S_s. [from: Yann-Edwin Keta et al. "Collective motion in large deviations of active particles". In: *arXiv preprint arXiv:2009.07112* (2020)]

$\rightarrow$ small-q limit not apparent

$\Rightarrow$ density fluctuations suppressed for $s < 0$

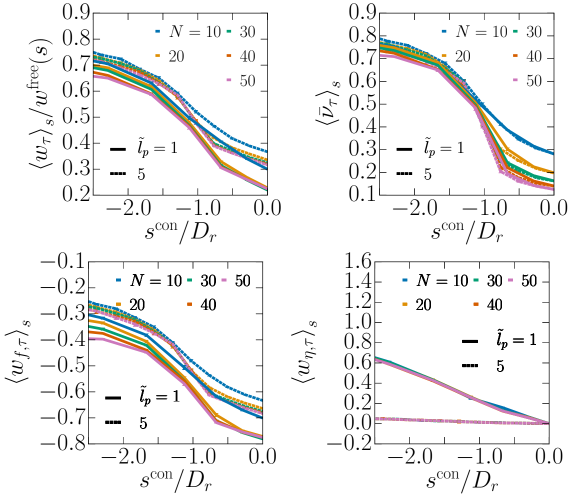


Figure: Biased averages of the polarisation $\langle \bar{\nu}_\tau \rangle_s$, the active work $\langle w_\tau \rangle_s$ and its force $\langle w_{f,\tau} \rangle_s$ and noise part $\langle w_{\eta,\tau} \rangle_s$. [from: Yann-Edwin Keta et al. "Collective motion in large deviations of active particles". In: *arXiv preprint arXiv:2009.07112* (2020)]

$\rightarrow$ isotropic mechanism to produce large deviations of w_τ