

Polarisation-biased trajectories of independent Brownian rotors

Analytic considerations with Mathieu functions

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I. SCALED CUMULANT GENERATING FUNCTION AND RATE FUNCTION

We wish to bias the trajectories of the system with respect to the mean vectorial polarisation over a trajectory,

$$\mathbf{p}_\tau = \frac{1}{\tau} \int_0^\tau dt \mathbf{p}(t) = \frac{1}{N\tau} \int_0^\tau dt \sum_i \mathbf{u}(\theta_i(t)), \quad (1)$$

and therefore need to compute the scaled cumulant generating function (SCGF)

$$N\psi_{\mathbf{p}}(\mathbf{s}) = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \log \left\langle \exp \left(-\mathbf{s} \cdot N \int_0^\tau dt \mathbf{p}(t) \right) \right\rangle_0 \quad (2)$$

where we will assume that \mathbf{s} is along the x -axis, and compute

$$\psi_p(s) = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \log \left\langle \exp \left(-sN \int_0^\tau dt p_x(t) \right) \right\rangle_0, \quad (3)$$

from which we can recover

$$\psi_{\mathbf{p}}(\mathbf{s}) = \psi_p \left(\sqrt{s_x^2 + s_y^2} \right) \quad (4)$$

from the fact that $\psi_{\mathbf{p}}(\mathbf{s})$ has to be cylindrically symmetric. We then have that $N\psi_s(p)$ is the largest eigenvalue of the eigenproblem

$$N\psi_p(s)P[\{\theta_i\}] = \mathcal{W}_{s,p}P[\{\theta_i\}], \quad (5)$$

where we introduced the tilted generator [1]

$$\mathcal{W}_{s,p} = \mathcal{L} - sNp = D_r \sum_i \frac{\partial^2}{\partial \theta_i^2} - s \sum_i \cos \theta_i, \quad (6)$$

using here $s \equiv s_x$ and $p \equiv p_x$, so that

$$\sum_i \left(\prod_{j \neq i} P(\theta_j) \right) \left[\psi_p(s)P(\theta_i) - \left(D_r \frac{\partial^2}{\partial \theta_i^2} P(\theta_i) - s \cos(\theta_i)P(\theta_i) \right) \right] = 0, \quad (7)$$

is equivalent to the 1-particle eigenproblem,

$$\psi_p(s)P(\theta) - \left(D_r \frac{\partial^2}{\partial \theta^2} P(\theta) - s \cos \theta P(\theta) \right) = 0 \Leftrightarrow \frac{\partial^2}{\partial \theta^2} \tilde{P}(\theta') + (a - 2q \cos 2\theta') \tilde{P}(\theta') = 0, \quad (8)$$

with $2\theta' = \theta$, $\tilde{P}(\theta/2) = P(\theta)$, and

$$a = -\frac{4\psi_p(s)}{D_r}, \quad q = \frac{2s}{D_r}, \quad (9)$$

and which solutions are known as the Mathieu functions [2].

Most notably, we have that for any $q \in \mathbb{R}$ there is a countable infinity of a . Inspired by [3] we will choose $a_{\text{Mathieu},0}(q)$ the characteristic value of the 0-th Mathieu function which is π -periodic and even. We thus have the SCGF

$$N\psi_{\mathbf{p}}(\mathbf{s}) = N\psi_p \left(\sqrt{s_x^2 + s_y^2} \right) = -N \frac{D_r}{4} a_{\text{Mathieu},0} \left(\frac{2}{D_r} \sqrt{s_x^2 + s_y^2} \right), \quad (10)$$

and by Legendre transform

$$\begin{aligned} NI(\mathbf{p}) &= \sup_{\mathbf{s} \in \mathbb{R}^2} \{-\mathbf{s} \cdot N\mathbf{p} - N\psi_{\mathbf{p}}(\mathbf{s})\} \\ &= \sup_{\mathbf{s} \in \mathbb{R}^2} \left\{ -\mathbf{s} \cdot N\mathbf{p} + N \frac{D_r}{4} a_{\text{Mathieu},0} \left(\frac{2}{D_r} \sqrt{s_x^2 + s_y^2} \right) \right\}, \end{aligned} \quad (11)$$

we obtain the rate function. We note that both $\psi_{\mathbf{p}}(\mathbf{s})$ and $I(\mathbf{p})$ are cylindrically symmetric.

We have the following expansion of the SCGF for small s [4],

$$\begin{aligned} \psi_{\mathbf{p}}(\mathbf{s}) &= -\frac{D_r}{4} \left(-\frac{1}{2} \left(\frac{2}{D_r} \sqrt{s_x^2 + s_y^2} \right)^2 + \mathcal{O}(|\mathbf{s}|^4) \right), \quad s \rightarrow 0 \\ &= \frac{1}{2} (s_x^2 + s_y^2) \frac{1}{D_r} + \mathcal{O}(|\mathbf{s}|^4), \quad s \rightarrow 0, \end{aligned} \quad (12)$$

and thus with

$$\begin{aligned} \left(\frac{\partial^2}{\partial s_x^2} + \frac{\partial^2}{\partial s_y^2} \right) \psi_{\mathbf{p}}(\mathbf{s}) &= N\tau \left(\langle p_{x,\tau}^2 + p_{y,\tau}^2 \rangle_{\mathbf{s}} - \langle p_{x,\tau} \rangle_{\mathbf{s}}^2 - \langle p_{y,\tau} \rangle_{\mathbf{s}}^2 \right) = N\tau \left(\langle \mathbf{p}_{\tau}^2 \rangle_{\mathbf{s}} - \langle \mathbf{p}_{\tau} \rangle_{\mathbf{s}}^2 \right) \\ &= N\tau \text{Var}(\mathbf{p}_{\tau})_{\mathbf{s}}, \end{aligned} \quad (13)$$

we get

$$\text{Var}(\mathbf{p}_{\tau})_0 = \frac{2}{N\tau D_r}, \quad (14)$$

and thus

$$\begin{aligned} I(\mathbf{p}) &= \frac{1}{2} \mathbf{p} \cdot \begin{pmatrix} \left. \frac{\partial^2 I}{\partial p_x^2} \right|_0 & \left. \frac{\partial^2 I}{\partial p_x \partial p_y} \right|_0 \\ \left. \frac{\partial^2 I}{\partial p_x \partial p_y} \right|_0 & \left. \frac{\partial^2 I}{\partial p_y^2} \right|_0 \end{pmatrix} \mathbf{p} + \mathcal{O}(\mathbf{p}^4) \\ &= \frac{1}{2} D_r \mathbf{p}^2 + \mathcal{O}(\mathbf{p}^4), \end{aligned} \quad (15)$$

the rate function (see Fig. 1 **(left)**), considering $I(0) = 0$ and $I(\mathbf{p}) = I(-\mathbf{p})$.

We can compare the rate function to numerical results from the cloning simulations of Brownian rotors biased with respect to their squared polarisation, and the semi-analytical upper bound $-\inf_s \tilde{B}_{s,p^2}$ obtained in this case [5] (see Fig. 1 **(centre)**).

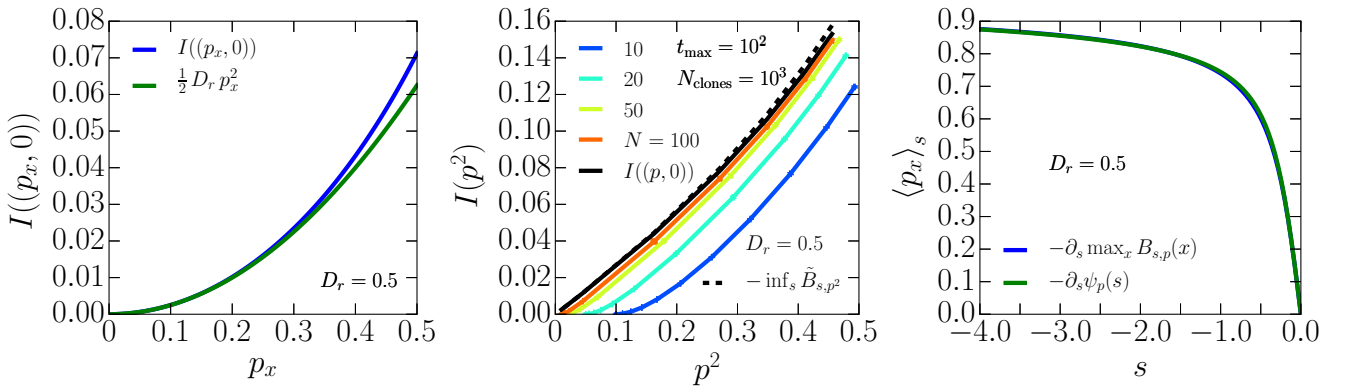



FIG. 1: **(left)** Rate function. – Using MATHIEU in  yketa/active_work/rotors.py. **(centre)** Comparison to numerics – $N_{\text{clones}} = 10^3$, $t_{\text{max}} = 10^2$. **(right)** Biased average of the polarisation along the x-axis.

II. OPTIMAL CONTROL POTENTIAL

We have that the tilted generator is self-adjoint (hermitian), so that the left and right eigenfunctions are identical. We thus have the eigenfunction for the $\mathbf{s} \parallel \mathbf{e}_x$ problem,

$$\mathcal{F}_s(\theta) \propto y_{\text{Mathieu},0} \left(\frac{\theta}{2}, \frac{2s}{D_r} \right) \quad (16)$$

with $y_{\text{Mathieu},0}$ the 0-th Mathieu function, even and π -periodic, so that $\mathcal{F}_s(\theta)$ is 2π -periodic, associated to the eigenvalue $\psi_p(s)$. We can thus compute the optimal control potential [6]

$$\phi_s(\theta) = -2 \log \mathcal{F}_s(\theta) \quad (17)$$

to achieve the fluctuations characteristic to the biased trajectories. We can compute the curvature of this potential at

$$\theta = 0$$

$$\left. \frac{\partial^2}{\partial \theta^2} \phi_s(\theta) \right|_{\theta=0} = 2 \left(\mathcal{F}(\theta=0)^{-2} \left(\frac{\partial}{\partial \theta} \mathcal{F}(\theta=0) \right)^2 - \mathcal{F}(\theta=0)^{-1} \frac{\partial^2}{\partial \theta^2} \mathcal{F}(\theta=0) \right), \quad (18)$$

where

$$\frac{\partial}{\partial \theta} \mathcal{F}(\theta=0) = 0, \quad (19)$$

by parity of $y_{\text{Mathieu},0}$, and

$$\begin{aligned} -\mathcal{F}(\theta=0)^{-1} \frac{\partial^2}{\partial \theta^2} \mathcal{F}(\theta=0) &= -y_{\text{Mathieu},0} \left(\frac{\theta}{2}, \frac{2s}{D_r} \right)^{-1} \frac{\partial^2}{\partial \theta^2} y_{\text{Mathieu},0} \left(\frac{\theta}{2}, \frac{2s}{D_r} \right) \Big|_{\theta=0} \\ &= \frac{1}{4} \left(a_{\text{Mathieu},0} \left(\frac{2s}{D_r} \right) - 2 \frac{2s}{D_r} \right) \end{aligned} \quad (20)$$

from the differential equation defining $y_{\text{Mathieu},0}$ (Eq. (8)), therefore

$$\left. \frac{\partial^2}{\partial \theta^2} \phi_s(\theta) \right|_{\theta=0} = \frac{1}{2} \left(a_{\text{Mathieu},0} \left(\frac{2s}{D_r} \right) - 2 \frac{2s}{D_r} \right), \quad (21)$$

so we can compare this optimal potential to a potential $\phi_s^{(g)} \propto g(1 - \cos \theta)$,

$$\phi_s^{(g)}(\theta) = \frac{1}{2} \left(a_{\text{Mathieu},0} \left(\frac{2s}{D_r} \right) - 2 \frac{2s}{D_r} \right) (1 - \cos \theta), \quad (22)$$

of identical curvature at $\theta = 0$ (see Fig. 2 **(left)**).

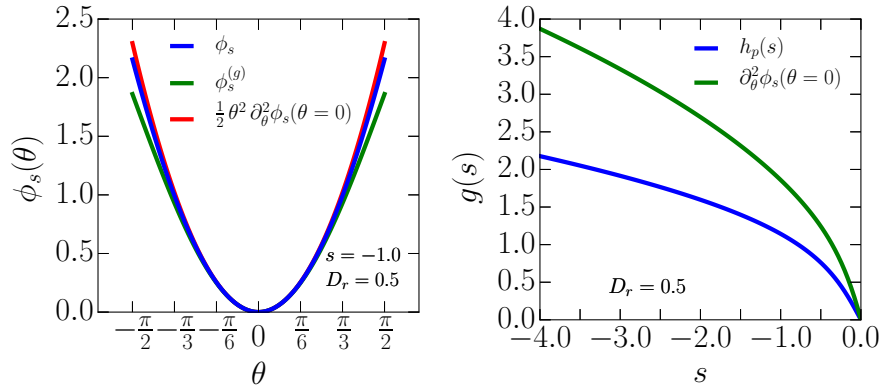



FIG. 2: **(left)** Optimal control potential. **(Right)** Torque parameter. – Using MATHIEU in  yketa/active_work/rotors.py.

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