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,

$$\boldsymbol{p}_\tau = \frac{1}{\tau}\int_0^\tau \mathrm{d}t\,\boldsymbol{p}(t) = \frac{1}{N\tau}\int_0^\tau \mathrm{d}t\,\sum_i \boldsymbol{u}(\theta_i(t)), \tag{1}$$

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

$$N\psi_{\boldsymbol{p}}(\boldsymbol{s}) = \lim_{\tau\to\infty}\frac{1}{\tau}\log\left\langle \exp\left(-\boldsymbol{s}\cdot N\int_0^\tau \mathrm{d}t\,\boldsymbol{p}(t)\right)\right\rangle_0 \tag{2}$$

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

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

from which we can recover

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

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

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

where we introduced the tilted generator [1]

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

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

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

is equivalent to the 1-particle eigenproblem,

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

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

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

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 $a_{\mathrm{Mathieu},0}(q)$ the characteristic value of the 0-th Mathieu function which is π-periodic and even. We thus have the SCGF

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

and by Legendre transform

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

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

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

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

and thus with

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

we get

$$
\mathrm{Var}(\boldsymbol{p}_\tau)_0 = \frac{2}{N\tau D_r}, \tag{14}
$$

and thus

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

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

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)**).

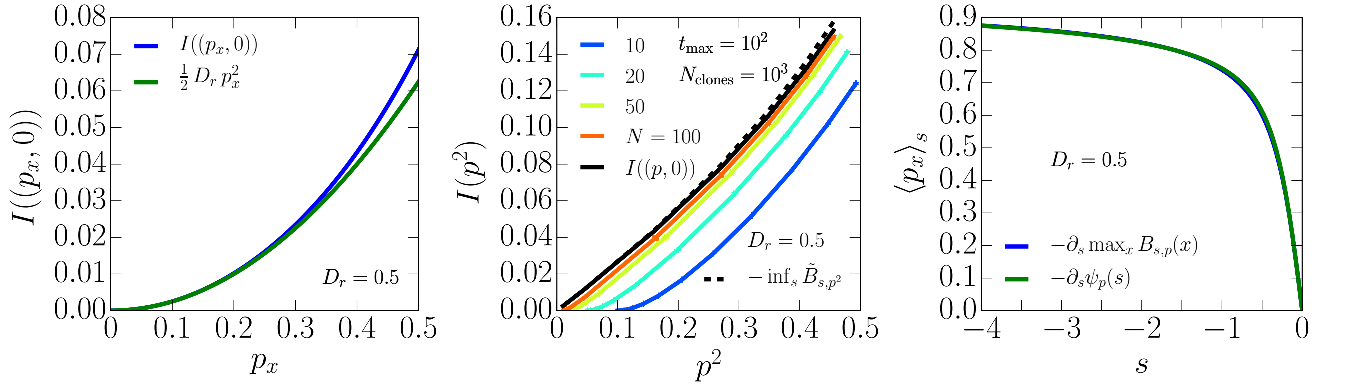

FIG. 1: **(left)** Rate function. – Using Mathieu in yketa/active_work/rotors.py. **(centre)** Comparison to numerics – $N_{\text{clones}} = 10^3$, $t_{\max} = 10^2$. **(right)** Biased average of the polarisation along the x-axis.

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 $\boldsymbol{s} \parallel \boldsymbol{e}_x$ problem,

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

with $y_{Mathieu,0}$ 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]

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

to achieve the fluctuations characteristic to the biased trajectories. We can compute the curvature of this potential at $\theta = 0$,

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

where

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

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

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

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

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

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

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

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

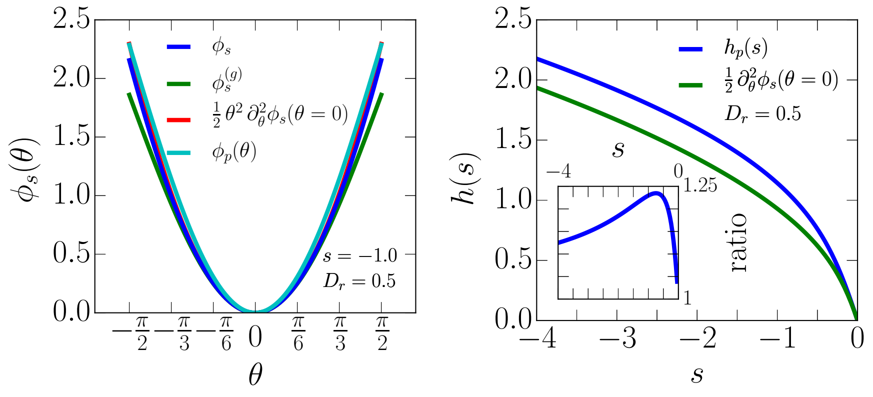

FIG. 2: **(left)** Optimal control potential. **(Right)** Torque parameter, where the factor 1/2 stems from Eq. (17). – Using MATHIEU in yketa/active_work/rotors.py.

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