

# Active Matter: from motility to self-organization

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## Exercises

### 1. MSD of a single Active Brownian Particle.

Consider a single APB with dynamics described by the equations

$$\begin{aligned}\partial_t \mathbf{r} &= v_0 \boldsymbol{\nu} + \sqrt{2D} \boldsymbol{\eta}, \\ \partial_t \theta &= \sqrt{2D_R} \eta_R,\end{aligned}$$

where  $\mathbf{r}$  is the center of mass of the particle. The ABP moves with a speed  $v_0$  along a unit vector  $\boldsymbol{\nu} = \cos \theta \hat{\mathbf{x}} + \sin \theta \hat{\mathbf{y}}$  that is pinned to its body axis. The self propulsion is not perfect in that it meanders a bit. This is captured by the  $\theta$  equation where  $\eta_R$  is a stochastic white noise that causes the direction to fluctuate.  $\boldsymbol{\eta}$  is the translational white noise that gives rise to diffusion. The noise has zero mean and correlations

$$\begin{aligned}\langle \eta_i(t) \eta_j(t') \rangle &= \delta_{ij} \delta(t - t') \\ \langle \eta_R(t) \eta_R(t') \rangle &= \delta(t - t')\end{aligned}$$

and all higher cumulants are zero, i.e., the noise is Gaussian. Our goal is to compute the MSD of the particle, i.e., derive Eq. (21) of the notes.  $\langle r_\alpha(t) r_\beta(t) \rangle$ .

(a) Show that

$$\langle \boldsymbol{\nu}(t) \boldsymbol{\nu}(t') \rangle = \frac{1}{2} \begin{pmatrix} \cos 2\theta_0 \exp(-D_R [t + t' + 2 \min(t, t')]) + \exp(-D_R [t + t' - 2 \min(t, t')]) & \sin 2\theta_0 \exp(-D_R [t + t' + 2 \min(t, t')]) \\ \sin 2\theta_0 \exp(-D_R [t + t' + 2 \min(t, t')]) & -\cos 2\theta_0 \exp(-D_R [t + t' + 2 \min(t, t')]) + \exp(-D_R [t + t' - 2 \min(t, t')]) \end{pmatrix}$$

- (b) Now compute  $\langle r_i(t) r_j(t) \rangle$  (assume  $\mathbf{r}(t=0) = 0$ ). You can average over the initial angle  $\theta_0$ .
- (c) Now analyze the form of the mean square displacement at short times i.e.,  $t \ll \frac{1}{D_R}$  and at long times, i.e.,  $t \gg \frac{1}{D_R}$ .
- (d) Write a program to evaluate numerically the MSD of a single APB neglecting the translational noise and compare your numerical result to your calculation, as well as to the MSD of a single overdamped Brownian particle.
- (e) Define an effective temperature  $T_{eff}$  for your ABP. Research the literature to find suitable parameters for, say, a typical Janus active colloid and evaluate  $T_{eff}$ .

### 2. Run-and-Tumble in 1D.

Consider  $N$  particles undergoing run-and-tumble dynamics in one dimension. These particles tumble at a constant rate  $\alpha$ , but their run speed  $v(x)$  is spatially varying. Such a situation can be achieved experimentally using, for instance, photokinetic *E. coli* [see G. Frangipane *et al.*, Dynamic density shaping of photokinetic *E. coli*, *eLife* **7**:e36608 (2018)]. Denote by  $R(x, t)$  and  $L(x, t)$  the density of right-moving and left-moving particles at time  $t$ .

- (a) Write Smoluchowski equations for the time evolution of  $R$  and  $L$ .
- (b) Reformulate the dynamics in terms of the total particle density  $\rho = R + L$  and their polarization  $p = R - L$ .
- (c) Show that the dynamics can be recast in the mean-field form given in Eqs. (??-??) and identify the expression for  $\mathcal{D}$ . Clearly state the approximations you need to make to obtain this form and discuss whether you think they may apply to the experiments of Frangipane *et al.*.
- (d) Find the steady state solution  $\rho_{ss}(x)$  of the equation you obtained in item 3 and contrast it to the steady state solution in the case where  $v = v_0$ .

## Open-ended Problems:

### 1. Mainly a literature search problem: Experimental observation of traveling waves or oscillations.

A very recent press release by Ramin Golestanian in Europhysics News highlights the rapidly growing interest in nonreciprocal interaction in non-equilibrium systems (<https://www.europhysicsnews.org/articles/epn/pdf/2024/03/epn2024553p12.pdf>).

Research the literature to identify an experimental system where traveling and/or oscillating states are observed and the dynamics can be mapped onto the NRCH model. Address the following questions:

- (a) Which are the coupled hydrodynamic fields at play in the system of your choice?
- (b) Why are they “hydrodynamics” (conserved fields, Goldstone modes, other)?
- (c) What are the physical mechanisms that engender effective NR interactions?
- (d) What are the experimental observations that may suggest NR interactions?
- (e) Do you think the system you have identified is a promising candidate for observing some of the predictions of NRCH models? What would you measure to establish the connection?

### 2. A data analysis problem.

In this Box folder <https://ucsb.box.com/s/6579eanfb8irrjnjd13aab0kphvyotxr> you will find the dataset data.tif. This is a tif stack of the spatio-temporal dynamics of the field  $\phi$  encoded as grayscale color values. The data were used to create Fig. 12 of F. Brauns and M. C. Marchetti, Phys. Rev. X **14**, 021014 (2024). Below I use the notation of that paper.

The simulation was run with parameters  $\tilde{D} = 0.3, D_{22} = 0.1, D_{11} = -1, \kappa = 1$ , on a square domain with periodic boundary conditions and side length  $L = 400$ . Snapshots were saved every 200 time units.

Suggested analysis:

- (a) Basic: Threshold and segment the images to analyze droplet morphologies (area, perimeter, tortuosity) and their statistics. (Use Mathematica’s Mathematical Morphology functionality <https://reference.wolfram.com/language/guide/MathematicalMorphology.html> or equivalent functionality in python or Matlab).

- (b) Advanced: Use PIV or optical flow analysis (e.g. using the PIVlab plugin in Matlab, OpenPIV in Python, or Mathematica's ImageDisplacements function) to find the droplet velocity field. Analyze the velocity fluctuations and correlations.
- (c) Bonus: Based on the PIV velocity fields, you can track droplets. The main challenge here is to account for droplet splitting and merging. How does the splitting rate of a droplet depend on its size? Can you come up with a stochastic model that describes the splitting and merging dynamics to reproduce the observed droplet size statistics?