Han summer school - homework

June 14, 2022

Active Brownian particle

Consider an active Brownian particle in two dimensions, following the overdamped Langevin equations of motion

$$\zeta \dot{\mathbf{r}} = F_{\mathrm{act}} \hat{\mathbf{n}} + \boldsymbol{\eta}^T \tag{1}$$

$$\dot{\theta} = \eta^r, \quad \hat{\mathbf{n}} = (\cos\theta, \sin\theta) \tag{2}$$

where F_{act} is the active force, η^T are the thermal fluctuations and η^r is rotational diffusion. Write a program to simulate such a particle in space and time, and extract its full trajectory data $x(t)$, $y(t)$ and $\theta(t)$. This is not very computationally intensive and your program should run in under a minute if written e.g. in python.

To do this effectively, we will work in simulation units. We choose a particle of radius 1, and we divide the first equation through by ζ. We then define the active velocity $v_0 = F_{\mathrm{act}}/\zeta$, and the rescaled thermal noise $\tilde{\boldsymbol{\eta}}^T = \boldsymbol{\eta}^T/\zeta$. Using the fluctuation-dissipation theorem, the thermal noise has mean 0 and its x and y components separately have a variance $\langle (\tilde{\boldsymbol{\eta}}_i^T)^2 \rangle = 2k_bT/\zeta$. We will assume that this is also 2, i.e. units where we measure energies in units of k_bT. Finally, we draw the rotational diffusion η^r from a Gaussian distribution with mean 0 and variance $2D_r$.

Use the slides on numerical simulations from the course material to implement your program. Then plot the trajectory for a couple of realisations of the system at different v_0 and D_r.

Use this information to compute several statistical quantities:

1. The angular mean square displacement, $\langle (\theta(t) - \theta(0))^2 \rangle$. What is its scaling and prefactor?

2. The full mean square displacement $\langle (\mathbf{r}(t) - \mathbf{r}(0))^2 \rangle$. Compare it to its theoretical prediction as a function of time, D_r and v_0.

Finally, to see much prettier ABP trajectories and MSDs, repeat your simulation for a system with zero temperature, i.e. where the thermal noise amplitude $\tilde{\boldsymbol{\eta}}_i^T = 0$.

Tip: To get better statistical results for your MSD, use a sliding window and the fact that things are time-translation invariant. Concretely, you want to average over all t_0 in your dataset where you can compute $\mathbf{r}(t + t_0) - \mathbf{r}(t_0)$, i.e. as long as $t + t_0$ is shorter than the simulation time.