Chapter 8

Living Crystals

Activity is commonly found in Nature as micro organisms utilize energy to perform directed motion to search for nutrients or avoid toxics. This has driven the interest of the scientific community in the study of active matter [1, 2]. Active Brownian particles are subject to similar conditions like Brownian particles, but they are also able to propel themselves in order to have a directed motion. As active systems are intrinsically out of equilibrium, phenomena that cannot be observed in a thermal equilibrium system emerge with activity [3]. Furthermore, experimentalists have also been motivated and inspired by natural swimmers to develop artificial ones [4, 5, 6, 7]. Such artificial microswimmers have been a fundamental tool to realize and study active matter, as well as to develop applications with a great potential for micro-transportation and nano-machinery [3, 8]. In this exercise, you are going to realize a many-body active matter system where particles interact according to aligning interactions [9]. This model studies how microswimmers interact when they get close to each other and how this results in crystal formation in an active environment. You will start with a simple simulation of active Brownian motion [10], then you will study a many-body system and see how these particles interact.

You will first consider a single Brownian particle that has a constant swimming velocity. This particle is subject to collisions from surrounding water molecules,
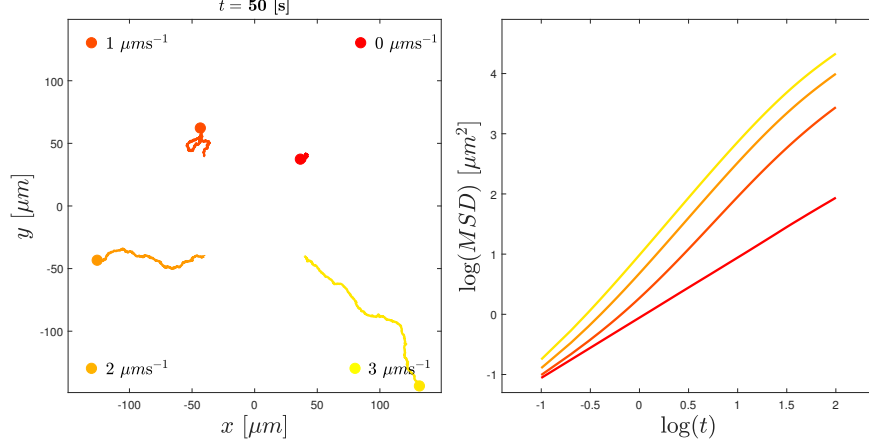
Figure 8.1: **Active Brownian Movement and displacement characteristics** (a) Sample trajectories of active Brownian particles with different swimming velocities. (b) Corresponding mean square displacements of the particles. Note that there is a super-diffusive regime for the active particles.

which creates diffusion. Alignment of this active particle will also fluctuate due to these collisions, which is called rotational diffusion. Overall, the equation of motion of this particle can be given as:

$$\frac{dx(t)}{dt} = v\cos\phi(t) + \sqrt{2D_T}W_x \tag{8.1}$$

$$\frac{dy(t)}{dt} = v\sin\phi(t) + \sqrt{2D_T}W_y \tag{8.2}$$

$$\frac{d\phi(t)}{dt} = \sqrt{2D_R}W_\phi \tag{8.3}$$

where v is the swimming velocity, ϕ is the instantaneous alignment and D_T, D_R are translational and rotational diffusion coefficients, respectively. W_x, W_y and W_ϕ are independent random numbers with mean zero and variance 1. Initially, we consider a single Brownian particle that moves in an environment with no net torque acting on it. Such a set of stochastic differential equations will yield different results in each realization, but some common characteristics can be found by averaging over many realizations. One of the most important feature of this motion is the mean-square-displacement:

$$\text{MSD}(\tau) = \langle [x(t+\tau) - x(t)]^2 + [y(t+\tau) - y(t)]^2 \rangle \tag{8.4}$$

44

You can see some sample trajectories in Figure 1(a) and corresponding mean square displacements in Figure 1(b). Note that the active swimming results in a super-diffusive behaviour in certain time scales, which means that the slope of the log(MSD) vs log(t) graph is greater than 1. Go through [10] for more detailed information.

In the next step, you will have a system of active Brownian particles that interact in an environment. First, you will focus on how these particles interact with each other and form metastable clusters [11]. Then, you will consider active particles that swim in an environment of densely packed passive particles and study formation of channels by active agents. Particle-particle interactions can be represented with the following interaction model: Each active particle n is subject to a torque due to all other particles; therefore, overall torque on each particle can be given by the following expression:

$$T_n = T_0 \sum_{i \neq n} \frac{\hat{v}_n \cdot \hat{r}_{ni}}{r_{ni}^2} \hat{v}_n \times \hat{r}_{ni} \cdot \hat{e}_z \quad \text{for} \quad r_{ni} < r_c \tag{8.5}$$

where T_0 represents the strength of interaction, $\hat{v}_n$ is the unit vector of the nth particle velocity and $\hat{r}_{ni}$ is the interparticle distance. A slightly different interaction plays a role if passive particles exist in the environment:

$$T_n = T_0 \sum_{i \neq n} \frac{\hat{v}_n \cdot \hat{r}_{ni}}{r_{ni}^2} \hat{v}_n \times \hat{r}_{ni} \cdot \hat{e}_z \tag{8.6}$$

$$- \sum_m \frac{\hat{v}_n \cdot \hat{r}_{nm}}{r_{nm}^2} \hat{v}_n \times \hat{r}_{nm} \cdot \hat{e}_z \quad \text{for} \quad r_{ni}, r_{nm} < r_c \tag{8.7}$$

Differently from active-active interactions, the interaction between active and passive particles has the opposite sign, therefore, a swimming particle will tend to align itself away from the passive one. This model is able to produce phenomenologically similar behaviours [9] to observation in the real world [11].

Exercises:

1. Implement the active Brownian motion simulation and reproduce some sample trajectories with different rotational diffusion constants. **To demonstrate (5 points)**: Results with a plot that shows (a) sample trajectories with different values of swimming velocity and (b) mean square displacement resulting from each trajectory. Present a result similar to Fig.1

2. Implement the many body model. Have at least 100 interacting particles. **To demonstrate (10 points)**: obtain individual clusters and plot some sample screen shots of the simulation with different cluster sizes. Prepare an animated video like the sample video (https://iopscience.iop.org/1367-2630/19/11/115008/media/njpaa9516video1.mp4).

3. Now try to include passive particles in a densely packed environment. Create the model and find correct parameters to observe metastable channels. **To demonstrate (10 points)**: Present your phenomenon with a video, like the sample video (https://iopscience.iop.org/1367-2630/19/11/115008/media/njpaa9516video2.mp4).

Bibliography

[1] S. Ramaswamy, "The mechanics and statistics of active matter," *Annu. Rev. Condens. Matter Phys.*, vol. 1, no. 1, pp. 323–345, 2010.

[2] P. Romanczuk, M. Bär, W. Ebeling, B. Lindner, and L. Schimansky-Geier, "Active brownian particles," *The European Physical Journal Special Topics*, vol. 202, no. 1, pp. 1–162, 2012.

[3] C. Bechinger, R. Di Leonardo, H. Löwen, C. Reichhardt, G. Volpe, and G. Volpe, "Active particles in complex and crowded environments," *Reviews of Modern Physics*, vol. 88, no. 4, p. 045006, 2016.

[4] G. Volpe, I. Buttinoni, D. Vogt, H.-J. Kümmerer, and C. Bechinger, "Microswimmers in patterned environments," *Soft Matter*, vol. 7, no. 19, pp. 8810–8815, 2011.

[5] I. Buttinoni, G. Volpe, F. Kümmel, G. Volpe, and C. Bechinger, "Active brownian motion tunable by light," *Journal of Physics: Condensed Matter*, vol. 24, no. 28, p. 284129, 2012.

[6] J. R. Howse, R. A. Jones, A. J. Ryan, T. Gough, R. Vafabakhsh, and R. Golestanian, "Self-motile colloidal particles: from directed propulsion to random walk," *Physical review letters*, vol. 99, no. 4, p. 048102, 2007.

[7] H.-R. Jiang, N. Yoshinaga, and M. Sano, "Active motion of a janus particle by self-thermophoresis in a defocused laser beam," *Physical review letters*, vol. 105, no. 26, p. 268302, 2010.

[8] U. Seifert, "Stochastic thermodynamics, fluctuation theorems and molecular machines," *Reports on progress in physics*, vol. 75, no. 12, p. 126001, 2012.

[9] S. Nilsson and G. Volpe, "Metastable clusters and channels formed by active particles with aligning interactions," *New Journal of Physics*, vol. 19, no. 11, p. 115008, 2017.

[10] G. Volpe, S. Gigan, and G. Volpe, "Simulation of the active brownian motion of a microswimmer," *American Journal of Physics*, vol. 82, no. 7, pp. 659–664, 2014.

[11] J. Palacci, S. Sacanna, A. P. Steinberg, D. J. Pine, and P. M. Chaikin, "Living crystals of light-activated colloidal surfers," *Science*, vol. 339, no. 6122, pp. 936–940, 2013.