IRG2 Workshop: How to Model Active Matter with Particles & Fields

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1 Question 1: Active Brownian Particle

Active matter refers to systems whose constituents consume energy, often generating directed motion. This motion, combined with interactions between the constituents, gives rise to emergent collective behavior. In this problem, we will investigate the dynamics of a simple model for a single active particle in two spatial dimensions. We refer to our model particle as an "active Brownian particle" (ABP.) The particle is characterized by its position in 2D space $\mathbf{x}(t)$ and its orientation $\mathbf{p}(t) = (\cos\theta(t), \sin\theta(t))$. The particle propels itself along $\mathbf{p}$ (via some "microscopic" process of energy consumption whose details we ignore), resulting in an equation of motion:

$$\dot{\mathbf{x}}(t) = v_a \mathbf{p}(t), \tag{1}$$

where v_a is the self propulsion speed. We will characterize the dynamics of our ABP by its mean-squared displacement, $\langle x^2(t)\rangle \equiv \langle \mathbf{x}(t)\cdot\mathbf{x}(t)\rangle$, where the angle brackets $\langle\cdots\rangle$ denote an average over independent realizations of this ABP (i.e. over independent trajectories.)

Problem 1: Write $\langle x^2(t)\rangle$ in terms of $\mathbf{p}(t)$.

Problem 2: Your answer to Problem 1 should involve a *correlation function*, $\langle \mathbf{p}(s_1)\cdot\mathbf{p}(s_2)\rangle$. What is the value of this function when $s_1 = s_2$?

The "Brownian" in ABP refers to the fact that the orientation of the particle can change randomly in time, according to a Gaussian white noise process $W(t)$, characterized by $\langle W(t)\rangle = 0$, $\langle W(t)W(t')\rangle = \delta(t - t')$. The diffusive dynamics of the orientation is given by:

$$\dot{\theta}(t) = \sqrt{D_r}W(t), \tag{2}$$

where D_r is a rotational diffusion constant.

Problem 3: Without doing any math, what do you expect the value of the orientation correlation function will be when $|s_2 - s_1| \gg 0$?

One can show (**BONUS**: can you show it?) that this diffusive dynamics for the angle θ results in an orientation correlation function given by:

$$\langle \mathbf{p}(s_1) \cdot \mathbf{p}(s_2) \rangle = \exp\left(-|s_1 - s_2|/\tau\right), \tag{3}$$

where τ is a timescale that depends on D_r.

Problem 4: Use dimensional analysis to guess how τ depends on D_r. Sketch what a typical ABP trajectory of length t_{obs} would look like for $D_r^{-1} \gg t_{\text{obs}}$ and $D_r^{-1} \ll t_{\text{obs}}$.

If we plug Eq. 3 into the expression for $\langle x^2(t) \rangle$ that we derived in Problem 1, we find (**BONUS**: do the derivation yourself):

$$\langle x^2(t) \rangle = 2v_a^2\tau^2 \left(\frac{t}{\tau} + \exp\left(-t/\tau\right) - 1 \right). \tag{4}$$

Problem 5: In the long-time limit where $t \gg \tau$, the MSD of Eq. 4 can be written in the form $\langle x^2(t) \rangle = 2D_e t$. What is D_e?

Problem 6: In the short-time limit where $t \ll \tau$, the expression for the MSD can be written approximately as a polynomial in time. What is the leading order term of this polynomial? (Hint: use the fact that for small y, $\exp\left(-y\right) \approx 1 - y + y^2/2$.) Interpret your result physically. (What word would you use to describe this kind of motion?)

Problem 7: Suppose that we confine our ABP to a circle of radius R. Compared to a uniform probability distribution over the interior of the circle, what will the probability distribution of the ABP position look like when (i) $R/v_a \gg \tau$ and (ii) $R/v_a \ll \tau$?

2 Question 2: Active Matter Field Theory

2.1 Background

We were able to understand the physics of a single active Brownian particle with straightforward pencil-and-paper calculations. But the physics of many, interacting active particles is much more complicated. One way to get a theoretical grip on such collections of active particles is to develop what is called a "hydrodynamic" (field) theory. To formally construct such a theory, we identify some important microscopic field (a quantity defined at each point in space and in time) and "coarse-grain,", smoothing out high-frequency spatial and temporal variations. This procedure is illustrated schematically in Fig. 1 below for a number density field of a system of N particles. The coarse-graining procedure converts the microscopic density field $\rho_{\text{micro}}(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r}_i - \mathbf{r})$, which varies rapidly and discontinuously in space, into a smooth,[1] coarse-grained density field $\rho(\mathbf{r})$ which describes only large-scale density variations.

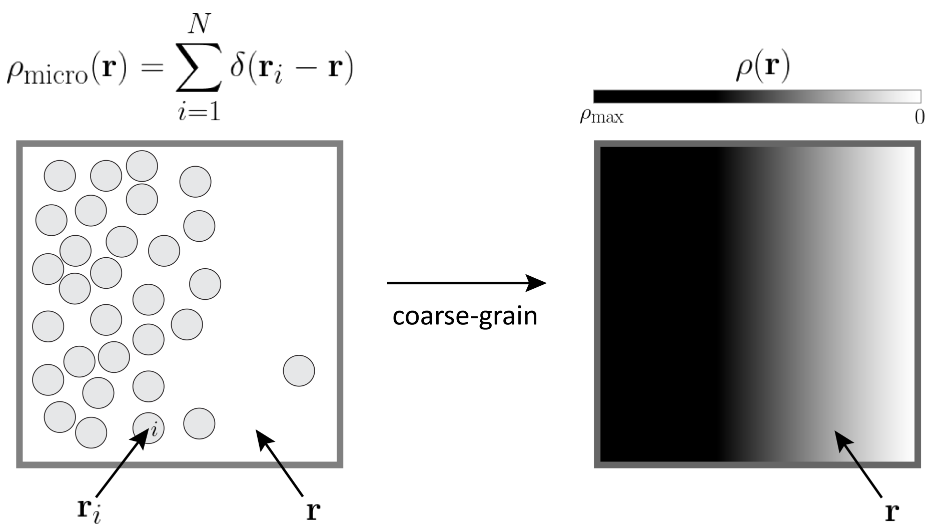


Figure 1: Schematic illustration of coarse-graining a density field.

Question: What sorts of fields would we need to describe the motion of a fluid?

In general, there are two kinds of hydrodynamic fields:

- Those corresponding to conserved quantities (e.g. mass.)
- Those corresponding to broken symmetries (e.g. translational or rotational.)

[1] The fact that the field is smooth is important because it allows us to take its derivatives, which is essential for mathematically constructing field theories.

The second kind of field is known as an *order parameter*. This quantity allows one to distinguish between ordered and disordered phases. For instance, in a nematic liquid crystal, rotational symmetry is broken. The corresponding order parameter (in 3D) is the Q tensor, $\mathbf{Q} = S(\hat{\mathbf{n}}\hat{\mathbf{n}} - (1/3)\mathbf{I})$ (where $\mathbf{I}$ is the 3x3 identity matrix) which quantifies the direction $\hat{\mathbf{n}}$ and magnitude S of the particles' orientation while respecting head/tail symmetry (see Fig. 2.)

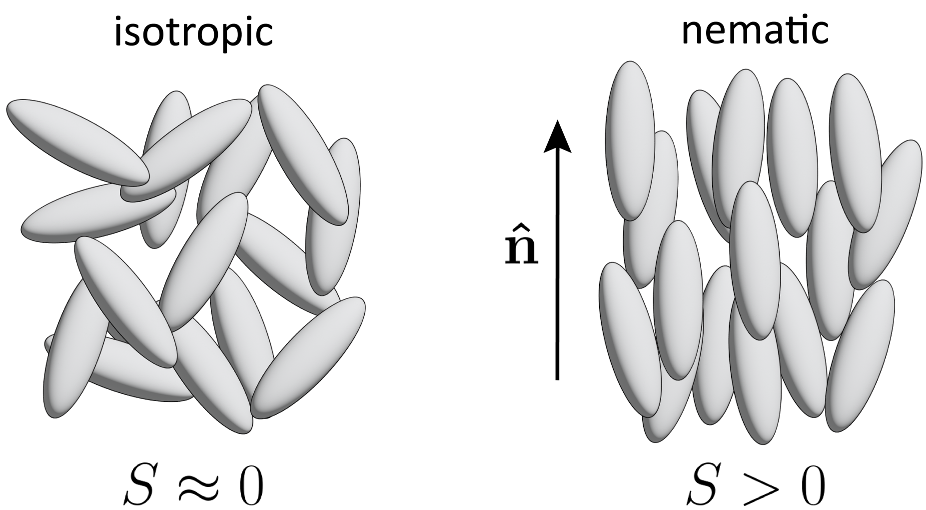


Figure 2: Illustration of isotropic and nematic liquid crystal phases. The scalar S is approximately zero in an isotropic phase, while it is between 0 and 1 in a nematic phase. The closer S is to 1, the more strongly the particles are oriented along the axis represented by the director, $\hat{\mathbf{n}}$.

Order parameters and the phases they describe can have symmetries. For example, nematic phases have head/tail symmetry (i.e. it doesn't matter whether we use $\hat{\mathbf{n}}$ or $-\hat{\mathbf{n}}$ to describe them.) On the other hand, a polar phase has distinct "head" and "tail" (or North and South, if you like) directions; the order parameter for such a phase is a vector, typically called the *polarization*.

In active systems, the self-propulsion force can also be either polar or nematic. The active Brownian particle of Question 1 has polar activity, since the self-propulsion force points in a specific direction. Other systems, like microtubules connected by ATP-consuming kinesin motors, have nematic activity (as the two microtubules are pushed or pulled in opposite directions by the motor.) See Fig. 3 for illustrations of the different kinds of order parameters and activities.

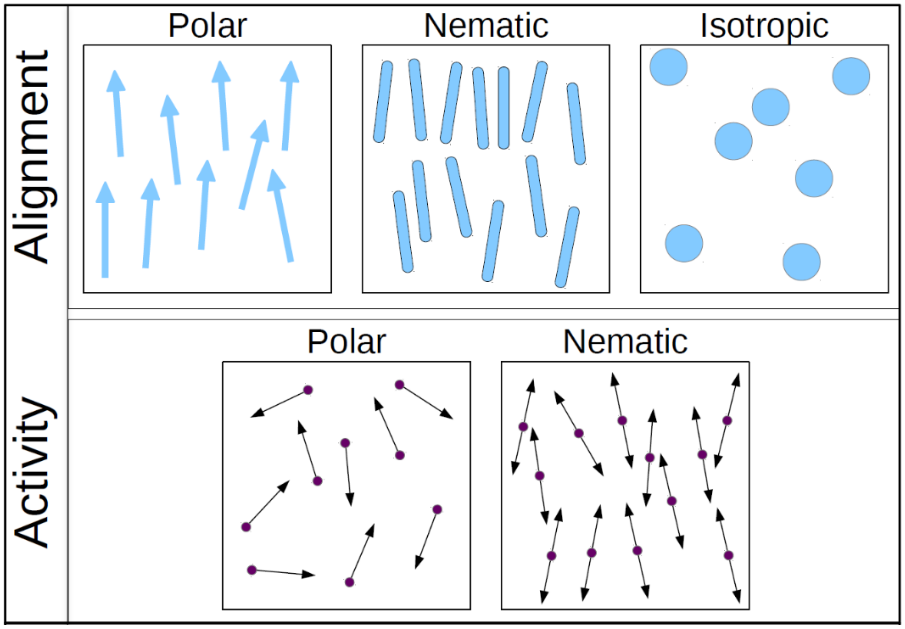
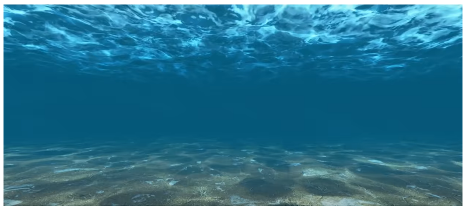


Figure 3: Illustration of different kinds of order (alignment) and activity. Modified from: M.F. Hagan & A. Baskaran, Curr. Opin. Cell Biol., 2016.

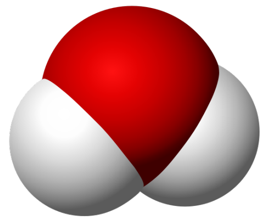
2.2 Your task

Below are images of several many-body systems, along with more detailed images of their "particle" constituents. Videos of each of these systems are also linked. For each system: (i) Identify any conserved quantities; (ii) Identify whether or not there is a broken symmetry (translational, rotational, ...) If so, identify the corresponding order parameter and state whether it is polar, nematic, or isotropic. (iii) If the system is active, decide whether the activity is polar or nematic. (Hint: systems 1 and 2 are passive, and the rest are active. System 1 has no broken symmetries; system 2 has no conserved quantities.)

BONUS: If you have time, try writing out the kinds of mathematical terms you would expect to see in a hydrodynamic theory for each system. (e.g., what sorts of quantities appear in the Navier-Stokes equations for water?)

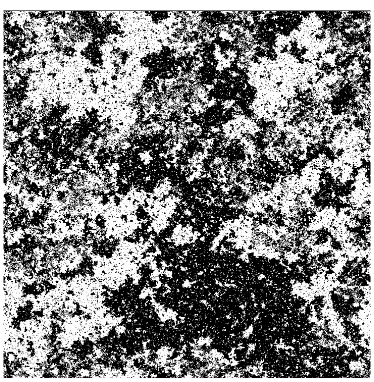


(a) Body of water.

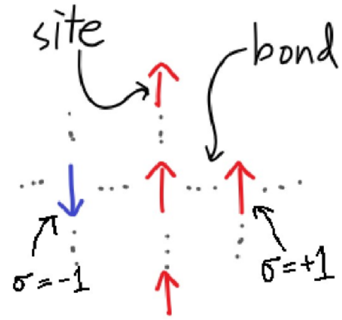


(b) Water molecule.

System 1: Water.
Video: https://youtu.be/kC0sLdh06aE.
Credit for panel a: see video. Credit for panel b: Wikipedia.

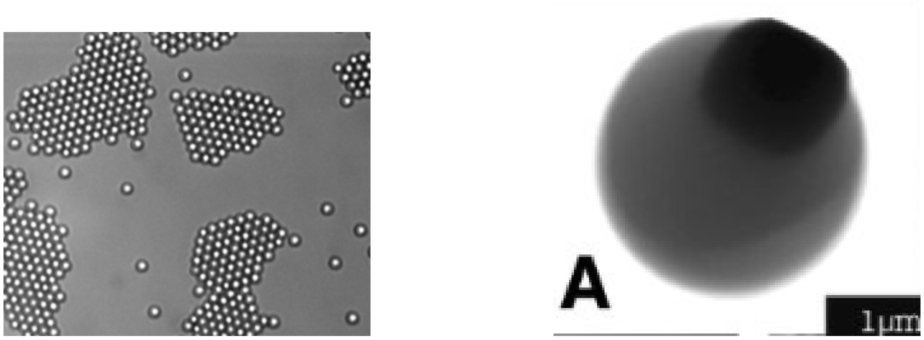


(a) A snapshot of an Ising model.



(b) An Ising spin and its nearest neighbors.

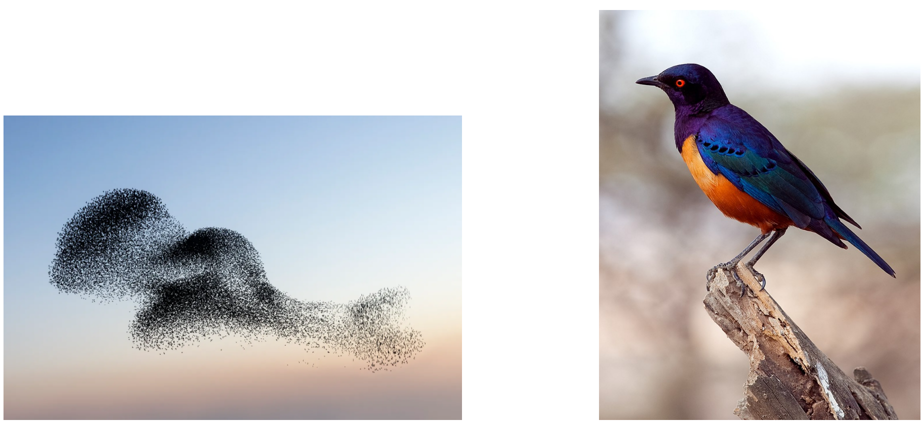
System 2: Ising model.
Video: https://youtu.be/kjwKgpQ-l1s.
Credit for panel a: https://condensedconcepts.blogspot.com/2018/09/what-can-students-learn-from-ising.html. Credit for panel b: https://stanford.edu/ jeffjar/statmech/intro4.html



(a) Snapshot of the light-activated colloids.

(b) A single light-activated colloid.

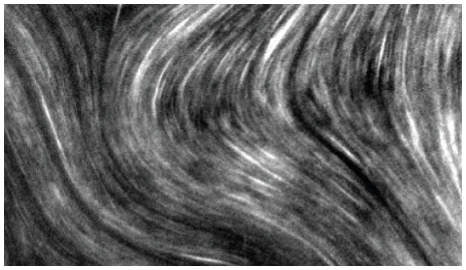
System 3: Light-activated active colloids.
Video: https://youtu.be/jqwOYh5hUlc.
Credit: https://www.science.org/doi/full/10.1126/science.1230020.



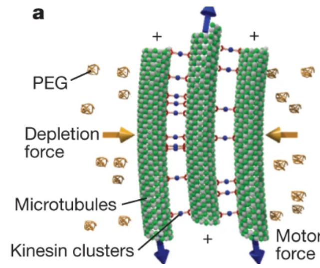
(a) Starling murmuration (flock.)

(b) A starling.

System 4: Flock of starlings.
Video: https://youtu.be/bb9ZTbYGRdc.
Credit for panel a: https://www.wired.com/story/stunning-images-of-starlings-in-flight/. Credit for panel b: Wikipedia.



(a) Microtubule + kinesin mixture confined to a fluid interface



(b) Microtubules with kinesin motors.

System 5: Dense suspension of microtubules, kinesin, and ATP.
Video: https://youtu.be/jny3Df6xn3w.
Credit: https://www.nature.com/articles/nature11591.

(a) A mosh pit.

(b) Closeup of some metal fans.

System 6: Heavy metal mosh pit.
Video: https://youtu.be/5jKU7gdxncE.
Credit for panel a: https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.110.228701.
Credit for panel b: https://www.popsci.com/article/science/psychology-loving-heavy-metal/.