# Theory of active materials

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## 1 Dynamics in thermal equilibrium: A crash course

### 1.1 The Langevin equation

Consider a small particle floating in a liquid such as, for concreteness sake, a colloid, that is a little glass or plastic bead of size of about  $1\mu m$ . What is its exact dynamics? You probably recall Brownian motion, but here we will derive it from first principles. As we are at scales and temperatures where quantum mechanics is irrelevant, we simply have Newton's equation:

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i,$$

where  $m_i$  is the mass of particle i at position  $\mathbf{r}_i$ , and  $\mathbf{F}_i$  is the total force acting on it.

The force has multiple components. First of all, since the particle is surrounded by a liquid, it will experience a drag force proportional to its velocity  $\mathbf{v}_i = \frac{d\mathbf{r}_i}{dt}$ ,  $\mathbf{F}^{\text{drag}} = -\zeta \mathbf{v}_i$ . For a spherical particle in laminar flow, the friction coefficient  $\zeta$  can be computed analytically and it is given by Stokes drag,  $\zeta = 6\pi\eta R$ , where  $\eta$  is the viscosity of the liquid and R is the particle radius. Second, there will be forces which arise from interacting with other particles j, which we will generically call  $\mathbf{F}_{ij}$ . There can also be external forces, such as with boundaries, or arising from gravity, which we will call  $\mathbf{F}_i^{\text{ext}}$ .

Most importantly, we need to consider the effect of being surrounded by water molecules at the microscopic scale, and constantly colliding with them. Molecules are much smaller than our particle (about 0.1nm), and collisions happen on a time scale much shorter than the particle motion (about  $10^{-14}s$ ). Therefore, we can approximate them as fluctuating random force  $\mathbf{f}_i^{\text{fluct}}$  that is uncorrelated in time and space, such that

$$\langle \mathbf{f}_i^{\text{fluct}} \rangle = 0, \quad \langle \mathbf{f}(t)_i^{\text{fluct}} \cdot \mathbf{f}(t')_j^{\text{fluct}} \rangle = 2d\Gamma \delta_{ij} \delta_{\alpha\beta} \delta(t - t'),$$
 (1)

where (for now) we introduce the constant  $\Gamma$ , and d is the dimension of space. Then we write:

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = -\zeta \frac{d\mathbf{r}_i}{dt} + \mathbf{F}_i^{\text{ext}} + \sum_j \mathbf{F}_{ij} + \mathbf{f}^{\text{fluct}}$$
 (2)

This is the **Langevin equation**, named after French physicist Paul Langevin, who derived it in the 1920s. The key difference with Newton's equation that this is a set of

stochastic ordinary differential equations due to the presence of fluctuating force.<sup>1</sup>

#### 1.2 Diffusion and the Stokes-Einstein relation

Let us consider the motion of a single particle under Langevin dynamics. We will assume that it has been density matched with the surrounding liquid, so that gravity is negligible, and that we are far from any walls. Then we would like to solve the equation

$$m\frac{d^2\mathbf{r}}{dt^2} = -\zeta \frac{d\mathbf{r}}{dt} + \mathbf{f}^{\text{fluct}} \tag{3}$$

Note that if we define the velocity variable  $\mathbf{v} = \frac{d\mathbf{r}}{dt}$ , this is now a first order stochastic ODE in the velocity, which we can write as

$$m\frac{d\mathbf{v}}{dt} + \zeta\mathbf{v} = \mathbf{f}^{\text{fluct}}.$$

We can solve this ODE using an integrating factor, and formally write

$$\mathbf{v}(t) = \mathbf{v}(0)e^{-t\zeta/m} + \frac{1}{m} \int_0^t e^{-(t-t')\zeta/m} \mathbf{f}^{\text{fluct}}(t')dt'. \tag{4}$$

The velocity is now a stochastic function, and we can immediately see that  $\langle \mathbf{v}(t) \rangle = \mathbf{v}(0)e^{-t\zeta/m}$ , so that in the long-time limit the average velocity is zero. This is consistent with Brownian motion where there is no average direction of motion. We introduce the ballistic time scale  $\tau_b = \frac{m}{\zeta}$  which controls the time over which the system forgets its initial velocity.

However, the mean-square velocity does not vanish: We can compute

$$\langle |\mathbf{v}(t)|^2 \rangle = \langle \mathbf{v}(t) \cdot \mathbf{v}(t) \rangle$$

$$= |\mathbf{v}(0)|^2 e^{-2t\zeta/m} + \frac{d\Gamma}{m\zeta} \left( 1 - e^{-2t\zeta/m} \right)$$

$$\to \frac{d\Gamma}{m\zeta} \quad \text{for } t \to \infty,$$

where d is the number of dimensions we work in (so typically d = 1, 2 or 3). This also makes sense as the particle is constantly fluctuating around its position. We can already link this to thermal equilibrium by noting that in equipartition, every degree of freedom contains  $\frac{1}{2}k_bT$  of energy. By linking this to the particle's kinetic energy, we write

$$\frac{1}{2}m\langle|\mathbf{v}(t)|^2\rangle = \frac{d\Gamma}{2\zeta} = \frac{d}{2}k_bT,$$

which leads us to identify

$$\Gamma = \zeta k_b T. \tag{5}$$

<sup>&</sup>lt;sup>1</sup>Strictly speaking, what we have written here is not fully general: particles moving past each other also interact through the fluid motion, and in principle we therefore need to use a friction matrix,  $\mathbf{F}^{\text{drag}} = -\sum_{j} \hat{\zeta}_{ij} \cdot \mathbf{v}_{j}$  that couples all particles. For the applications we consider here, this will rarely be relevant

This equation links the amplitude of the fluctuating force,  $\Gamma$  with the friction coefficient  $\zeta$  of the surrounding medium using  $k_bT$ . This is the simplest example of a **fluctuation-dissipation relation**, which is one of the hallmarks of thermal equilibrium.

Ultimately, we are interested in finding the trajectory of our particle, which we can formally write as

$$\mathbf{r}(t) = \mathbf{r}(0) + \int_0^t \mathbf{v}(t')dt'.$$

We can quickly see that on average, in the long-time limit  $\langle \mathbf{r}(t) \rangle = 0$ , i.e. we are going nowhere (we will set  $\mathbf{r}(0) = 0$  for convenience).

However, the fluctuations around this state are not zero, and with time we will move further and further away from the initial position. We measure how far we have diffused away from the origin as a function of time using the **mean square displacement** 

$$MSD(t) = \langle |\mathbf{r}(t) - \mathbf{r}(0)|^2 \rangle$$

$$= \dots \text{ lengthy calculation } \dots$$

$$= \frac{d\Gamma}{\zeta^2} \left[ 2t + \frac{m}{\zeta} \left( -2 + 2e^{-t\zeta/m} \right) \right]$$

$$\to \frac{2d\Gamma}{\zeta^2} t \quad \text{for } t \to \infty$$

$$(6)$$

$$(7)$$

The MSD is an interesting function: At short time scales, an expansion to second order in t reveals that  $MSD(t) \sim t^2$ . This is the ballistic regime where the particle goes nearly in a straight line, which is valid for  $t \leq \tau_b$ .

In the long-time limit, we have instead  $MSD(t) \sim t$ . This is the diffusive regime where the typical distance travelled by the particle goes as  $\sqrt{\langle |\mathbf{r}(t) - \mathbf{r}(0)|^2 \rangle} \sim t^{1/2}$ , i.e. it grows with the square root of time. We express this using the **diffusion coefficient** MSD(t) = 2Dt, and using the long-time limit of eq. 7 together with the fluctuation-dissipation relation eq. 5, we obtain the **Einstein relation** 

$$D = d\frac{k_b T}{\zeta} \tag{8}$$

that relates the diffusion coefficient to the temperature and the friction of the medium. In three dimensions, if we use the Stokes relation linking friction and viscosity for a spherical particle, we can write the **Stokes-Einstein relation** which is especially useful for colloids,

$$D = \frac{k_b T}{6\pi \eta R}. (9)$$

In the exercise associated to today's lecture, in addition to filling in the steps of this calculation, you will also estimate  $\tau_b$  and D numerically for different objects. For a colloid of  $1\mu m$  radius,  $\tau_b \sim 10^{-7} s$ , well below the diffusive time scale, which can be estimated by the time at which the MSD reaches the particle radius,  $R^2$ , which is several seconds.

As we can see, on time scales relevant to observable particle diffusion, we have gone long past the ballistic regime where the mass matters. Then, for  $t \gg \tau_b$ , we can considerably simplify our approach by simply neglecting the inertial term, and writing the **overdamped Langevin equation** 

$$\frac{d\mathbf{r}_i}{dt} = \mu \left[ \mathbf{F}_i^{\text{ext}} + \sum_j \mathbf{F}_{ij} \right] + \boldsymbol{\eta}_i, \tag{10}$$

where  $\mu = 1/\zeta$  is the particle mobility or inverse friction, and we have a new rescaled fluctuating force, the **thermal noise**  $\eta_i$  which follows the same fluctuation-dissipation law:

$$\langle \boldsymbol{\eta}_i(t) \cdot \boldsymbol{\eta}_j(t') \rangle = 2d \frac{k_b T}{\zeta} \delta_{ij} \delta(t - t').$$
 (11)

Note that this is very similar to taking the low Reynolds number limit in fluid dynamics to go from the Navier-Stokes equation to the Stokes equation. The overdamped Langevin equation will be the starting point for introducing microscopic active matter models, in particular active Brownian particles.

# 2 The Fokker-Planck equation

Later in the course, we will work on the continuum scale and extensively use **hydrody-namic equations**, which are for quantities like particle density, velocity and orientation. These two approaches are in fact formally linked to each other, and we will make use of this approach when we derive the continuum equations appropriate to active materials.

The Langevin equation (and more obviously its overdamped counterpart) can formally be written as

$$\frac{d\mathbf{A}}{dt} = \mathbf{V}(\mathbf{A}) + \boldsymbol{\eta},\tag{12}$$

where **A** is a vector of degrees of freedom  $\{\mathbf{r}_i, \mathbf{p}_i\}$  (positions and momenta of all the *N* particles), **V** is a generalised velocity that includes the deterministic forces and dissipative parts. Finally,  $\boldsymbol{\eta}$  contains the fluctuating components, such that  $\langle \boldsymbol{\eta} \rangle = 0$  and

$$\langle \boldsymbol{\eta}(t) \otimes \boldsymbol{\eta}(t') \rangle = 2\hat{\mathbf{B}}\delta(t - t').$$
 (13)

Let us now consider the joint probability density of finding my N particles at certain positions and momenta at time t,  $P_N(\mathbf{A}, t) \equiv P_N(\{\mathbf{r}_i, \mathbf{p}_i\}, t)$ . This is a function in 2dN dimensions, or in dN dimensions for the overdamped case.

Since none of my particles are either created or disappear, the total probability is conserved, i.e.  $\int d\mathbf{A} P_N(\mathbf{A}, t) = 1$ . We can then derive the time evolution of the probability density. Consider a finite volume  $V_0$  with boundary  $S_0$  in phase space. Then we have

$$\frac{\partial}{\partial t} \int_{V_0} d\mathbf{A} P_N(\mathbf{A}, t) = -\int_{S_0} P_N(\mathbf{A}, t) \frac{\partial \mathbf{A}}{\partial t} \cdot d\mathbf{S}_0,$$

where  $\frac{d\mathbf{A}}{dt}$  is the flux of  $\mathbf{A}$  through the surface defined by surface element  $\mathbf{S}_0$ . This is very analogous to Gauss' law in electromagnetism. We can then indeed use Gauss' theorem to convert the surface integral back to a volume integral and write

$$\int_{S_0} P_N(\mathbf{A}) \frac{\partial \mathbf{A}}{\partial t} \cdot d\mathbf{S}_0 = \int_{V_0} d\mathbf{A} \frac{\partial}{\partial \mathbf{A}} \left( \frac{\partial \mathbf{A}}{\partial t} P_N(\mathbf{A}, t) \right)$$

Putting both sides together and taking the size of  $V_0 \to 0$ , we have for the interior:

$$\begin{split} \frac{\partial P_N(\boldsymbol{A},t)}{\partial t} &= -\frac{\partial}{\partial \boldsymbol{A}} \left( \frac{\partial \boldsymbol{A}}{\partial t} P_N(\boldsymbol{A},t) \right) \\ &= -\frac{\partial}{\partial \boldsymbol{A}} \left( \boldsymbol{V} P_N(\boldsymbol{A},t) \right) - \frac{\partial}{\partial \boldsymbol{A}} \left( \boldsymbol{\eta} P_N(\boldsymbol{A},t) \right) \\ &:= -L_0 P_N(\boldsymbol{A},t) - L_1 P_N(\boldsymbol{A},t), \end{split}$$

where we have introduced the microscopic evolution equation 12 in the second step. In the last step, we have now separated out the probability flux into a deterministic part  $L_0$  and a stochastic part  $L_1$ . We need to do this since, ultimately, we want to get rid of the stochastic parts by taking a an average, i.e. want to compute  $\langle P_N(\mathbf{A},t)\rangle_{\boldsymbol{\eta}}$ . We proceed in stages. First, we can formally integrate out the deterministic part by defining  $P_N(\mathbf{A},t) = e^{-L_0t}\sigma(\mathbf{A},t)$ . Note that we require here that  $L_0$  depends only on the coordinate, and is not explicitly time-dependent. Then we can convince ourselves that the evolution of  $\sigma(\mathbf{A},t)$  has only stochastic pieces left:

$$\partial_t \sigma = L_0 e^{L_0 t} P_N + e^{L_0 t} \partial_t P_N$$
  
=  $L_0 e^{L_0 t} P_N + e^{L_0 t} (-L_0 P_N - L_1 P_N)$   
=  $-e^{L_0 t} L_1 e^{-L_0 t} \sigma := W(t) \sigma$ 

where we have defined the new stochastic process W(t) in the last step. Then, again, we can formally solve our equation and write  $\sigma(t) = e^{-\int_0^t dt' W(t')} \sigma(0)$ . Since W(t) is purely stochastic, we now need to be very careful in determining its properties. First of all, since  $\langle \boldsymbol{\eta} \rangle = 0$ , we also have  $\langle W(t) \rangle = 0$ . However, it is correlated in time,

$$\langle W(t_1)W(t_2)\rangle = e^{L_0 t_1} \frac{\partial}{\partial \mathbf{A}} \cdot \mathbf{\eta}(t_1) e^{L_0 t_2} \frac{\partial}{\partial \mathbf{A}} \cdot \mathbf{\eta}(t_2) e^{-l_0 t_2}$$
$$= \delta(t_1 - t_2) e^{L_0 t_1} \frac{\partial}{\partial \mathbf{A}} \cdot 2\hat{\mathbf{B}} \cdot \frac{\partial}{\partial \mathbf{A}} e^{-L_0 t_1}$$

Armed with this result, we can then carry out the stochastic average,

$$\langle \sigma(t) \rangle = \langle e^{-\int_0^t dt' W(t')} \rangle \sigma(0) = e^{-\frac{1}{2} \int_0^t \int_0^t dt_1 dt_2 \langle W(t_1) W(t_2) \rangle} \sigma(0),$$

where the second step is a general mathematical property of Gaussian variables (you may have seen it with operator exponentials in quantum mechanics). It can be shown by writing the exponential as a series and then using the fact that all odd moments average out to zero. We can then put all of our previous results together and find

$$\langle P_N(\boldsymbol{A},t)\rangle = e^{-L_0 t} e^{-\int_0^t dt_1 e^{L_0 t_1} \frac{\partial}{\partial \boldsymbol{A}} \cdot \boldsymbol{B} \cdot \frac{\partial}{\partial \boldsymbol{A}} e^{-L_0 t_1}} \sigma(0)$$

Finally, we can see that this equation is the solution to the differential equation<sup>2</sup>

$$\frac{\partial \langle P_N(\boldsymbol{A},t) \rangle}{\partial t} = -L_0 \langle P_N(\boldsymbol{A},t) \rangle + \frac{\partial}{\partial \boldsymbol{A}} \cdot \boldsymbol{B} \cdot \frac{\partial}{\partial \boldsymbol{A}} \langle P_N(\boldsymbol{A},t) \rangle. \tag{14}$$

This is the general form of the **Fokker Planck equation** for the evolution of the N-particle probability distribution. Despite its appealing form, it is in general not useful on its own as it still treats all of the degrees of freedom contained in  $\boldsymbol{A}$  explicitly. We will return to this point in lecture 3 on hydrodynamics.

# 2.1 The Smoluchowski equation, diffusion, and thermal equilibrium

For a single particle, or many non-interacting particles, the Fokker-Plank equation is however very useful, and we can relate it to our physics understanding of diffusion. Consider the overdamped Langevin equation for a particle in an external potential, for simplicity in one dimension:

$$\frac{dx}{dt} = -\frac{1}{\zeta} \frac{\partial V}{\partial x} + \frac{\xi}{\zeta}, \quad \langle \xi(t)\xi(t') \rangle = 2\zeta k_b T \tag{15}$$

We identify  $\mathbf{A} \equiv x$ ,  $\mathbf{V}(\mathbf{A}) \equiv -\frac{1}{\zeta} \frac{\partial V}{\partial x}$  and  $\mathbf{\eta} \equiv \xi/\zeta$ , with second moment  $\hat{\mathbf{B}} \equiv \frac{2k_bT}{\zeta}$ . Following the same steps as in the derivation above, we write the evolution equation for the probability density  $P_1(x,t)$  for the position of our particle in space as a function of time:

$$\frac{\partial P_1(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ \left( \frac{1}{\zeta} \frac{\partial V}{\partial x} + \eta \right) P_1(x,t) \right]$$

We identify the differential operators  $L_0 = \frac{\partial}{\partial x} \frac{1}{\zeta} \frac{\partial V}{\partial x}$  and  $L_1 = \frac{\partial}{\partial x} \eta$ . Then we can use the result that we just derived and write the Fokker-Planck equation for the probability density of my particle  $p(x,t) \equiv \langle P_1(x,t) \rangle$ 

$$\frac{\partial p(x,t)}{\partial t} = \frac{1}{\zeta} \frac{\partial}{\partial x} \left[ \frac{\partial V}{\partial x} p(x,t) \right] + \frac{k_b T}{\zeta} \frac{\partial^2 p(x,t)}{\partial x^2}.$$
 (16)

This is the **Smoluchowski equation** for the overdamped motion of a single particle in a potential.

We can immediately deduce a very important link: If we consider a system at low density where particles are approximately non-interacting, the density of particles  $\rho(x,t)$  is proportional to p(x,t) and follows the same equation. Using fluctuation-dissipation we also identify the diffusion coefficient  $D = k_b T/\zeta$ . Then if we then take a free system where V = 0, we recover the **diffusion equation** 

$$\frac{\partial \rho(x,t)}{\partial t} = D \frac{\partial^2 \rho(x,t)}{\partial x^2}.$$
 (17)

<sup>&</sup>lt;sup>2</sup>There are in general a number of well-hidden subtleties which we have glossed over in this derivation. We have implicitly used what is known as the Stratonovich convention for stochastic integration. Mathematicians prefer the Ito convention that treats discretisation slightly differently. Fortunately, in our case, they give the same result.

This is the continuum equivalent to the long-term diffusion motion for the single particle that we derived from the Langevin equation. Unfortunately, it is rare that we can make such a clean link between microscopic and continuum equations!

We can also now look at the first example of an important principle that we will repeatedly use for active materials: the idea of a **conserved current in response to a conservation law**. Here the conservation law is simply the conservation of density and the Smoluchowski equation can be written as a **continuity equation** 

$$\frac{\partial p(x,t)}{\partial t} = -\nabla \cdot \boldsymbol{J},\tag{18}$$

where J is the **conserved current** associated to the system. With a bit of rewriting, we find the (one-dimensional) density current

$$J = -\frac{1}{\zeta}p(x,t)\frac{\partial}{\partial x}\left[k_bT\ln p(x,t) + V\right]. \tag{19}$$

Then we can also recover **thermal equilibrium** in this framework: In equilibrium, we are in steady-state, i.e. there is no more explicit time dependence to the probability density,  $p(x,t) \equiv P_{\rm eq}(x)$  and  $\frac{\partial p(x,t)}{\partial t} = 0$ . This immediately gives us  $\nabla \cdot \boldsymbol{J} = 0$  and therefore  $\boldsymbol{J} = \boldsymbol{C}$ , a constant. If we require that at  $x \to \pm \infty$ , the probability vanishes (true if our system is in an arbitrarily large box), we find that J = 0 is the only solution. We can solve the resulting equation and write  $P_{\rm eq}(x) = Ae^{-V/k_bT}$ , where A is a constant. By requiring that the probability normalises to 1, we recover the equilibrium **Boltzmann distribution** 

$$P_{\text{eq}}(x) = \frac{1}{Z} e^{-V(x)/k_b T}, \quad Z = \int_{-\infty}^{\infty} dx e^{-V(x)/k_b T}.$$
 (20)

## References and further reading

- W. van Saarloos, V. Vitelli and Z. Zeravcic, *Soft Matter: Concepts, Phenomena, and Applications*, Princeton University Press (2024). This corresponds to the first part of chapter 3, but done a little more precisely.
- L.E. Reichl, A Modern Course in Statistical Physics, Wiley-WCH, 4th edition (2016). See chapter 7 for a somewhat more concrete treatment of the Fokker-Planck equation.
- M.C. Marchetti, *Hydrodynamics and active matter*, graduate course, Syracuse University (2012) (exists unfortunately only as a set of handwritten notes)
- M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics*, Clarendon Press (1988). The Brownian motion chapter is a more general version of the treatment here.

## 3 Active Brownian particles

From our discussion of equilibrium physics, we recall that we can write the **overdamped** Langevin equation in the limit of micron-size particles:

$$\frac{d\mathbf{r}_i}{dt} = \frac{1}{\zeta} \left[ \mathbf{F}_i^{\text{ext}} + \sum_j \mathbf{F}_{ij} \right] + \boldsymbol{\eta}_i, \tag{21}$$

where  $1/\zeta$  is the particle mobility or inverse friction. We have a fluctuating force, the **thermal noise**  $\eta_i$  which follows the fluctuation-dissipation relation

$$\langle \boldsymbol{\eta}_i(t) \cdot \boldsymbol{\eta}_j(t') \rangle = 2d \frac{k_b T}{\zeta} \delta_{ij} \delta(t - t').$$
 (22)

We will now make this an active system: Every one of our particles has a self-propulsion force  $\mathbf{F}_i^{\text{act}}$  that arises from biological processes such as for crawling cells or swimming bacteria. It could also represent the result of chemical processes such as electrophoresis or Marangoni flows that mace active colloids move. Regardless of the origin of the activity, we will approximate the active force as constant in magnitude  $F_i^{\text{act}} = \zeta v_0$ , where  $v_0$  is an active force. The direction it is pointing in will be denoted by the unit vector  $\hat{\mathbf{n}}_i$ , and we can then rewrite the overdamped Langevin equation as

$$\frac{d\mathbf{r}_i}{dt} = v_0 \hat{\boldsymbol{n}}_i + \frac{1}{\zeta} \sum_j \mathbf{F}_{ij} + \boldsymbol{\eta}_i. \tag{23}$$

The difference between the active force and an external force such as gravity is that  $\hat{n}_i$  is not a constant. We will stay in two dimensions for simplicity, though everything that follows exists in 3d, it is just unpleasantly technical to write down. Then we can parametrise it by an angle  $\theta_i$  as  $\hat{n}_i = (\cos \theta_i, \sin \theta_i)$ , and we can write down in full generality a Langevin evolution equation

$$\dot{\theta}_i = \frac{1}{\zeta_r} \sum_{ij} T_{ij} + \eta_i^r, \tag{24}$$

where  $T_{ij}$  are pair torques and  $\langle \eta_i^r(t) \eta_j^r(t') \rangle = 2D_r \delta_{ij} \delta(t-t')$  where  $D_r$  is a rotational diffusion constant. For an equilibrium system, one can derive a fluctuation-dissipation relation that shows that  $D_r = k_b T/\zeta_r$  in a way that is similar to what one does in class for translational diffusion. However, since these are active systems, fluctuations can also come from biological or chemical driving fluctuations, and so this does not need to be true.

The simplest model then is **Active Brownian motion** where  $T_{ij} = 0$ , and with fluctuations that do not necessarily follow fluctuation-dissipation:

$$\dot{\mathbf{r}}_i = v_0 \hat{\boldsymbol{n}}_i + \mu \sum_{ij} \mathbf{F}_{ij} + \boldsymbol{\eta}_i \tag{25}$$

$$\dot{\theta}_i = +\eta_i^r, \tag{26}$$

with  $\langle \boldsymbol{\eta}_i(t) \cdot \boldsymbol{\eta}_j(t') \rangle = 4D_t \delta_{ij} \delta(t-t')$  and  $\langle \eta_i^r(t) \eta_j^r(t') \rangle = 2D_r \delta_{ij} \delta(t-t')$  where D is a translational and  $D_r$  is a rotational diffusion constant.

## 3.1 A single Active Brownian particle (ABP)

Similar to what one does in equilibrium physics, we can solve the motion of a single ABP, i.e. the two coupled equations

$$\dot{\mathbf{r}} = v_0 \hat{\boldsymbol{n}} + \boldsymbol{\eta}, \quad \dot{\theta} = +\eta^r, \tag{27}$$

$$\langle \boldsymbol{\eta}(t) \cdot \boldsymbol{\eta}(t') \rangle = 4D_t \delta(t - t'), \quad \langle \eta^r(t) \eta^r(t') \rangle = 2D_r \delta(t - t') = \frac{2}{\tau_r} \delta(t - t'), \quad (28)$$

where  $\tau_r = 1/D_r$  will be the rotational persistence time.

We can solve this as follows: First formally integrate the angular equation of motion,

$$\theta(t) = \int_0^t \eta^r(t')dt',$$

As with thermal motion, we have zero average angle  $\langle \theta(t) \rangle = 0$ , but rotational diffusion  $\langle \theta(t)^2 \rangle = 2D_r t = \frac{2}{\tau_r} t$ . With some work, we can use this knowledge to compute the statistical properties of  $\hat{\boldsymbol{n}} = (\cos \theta, \sin \theta)$ : You need to expand the sine and cosine into a power series, and then compute all the moments. Since  $\theta$  has a Gaussian distribution, all the odd moments are zero, and all the even moments can be expressed as a function of  $\langle \theta(t)^2 \rangle$ . After resumming this series, one finds eventually:

$$\langle \hat{\boldsymbol{n}}(t) \rangle = 0, \tag{29}$$

$$\langle v_0 \hat{\boldsymbol{n}}(t) \cdot v_0 \hat{\boldsymbol{n}}(t') \rangle = 4 \frac{v_0^2 \tau_r}{2} \frac{1}{\tau_r} e^{-|t-t'|/\tau_r}, \tag{30}$$

i.e. the statistical properties of the active driving velocity  $v_0 \hat{\boldsymbol{n}}(t)$  act like a time-correlated noise with zero mean but time-correlated variance with correlation time  $\tau_r$ . This is sometimes called 'colored noise' or a 'memory kernel'. As shown in Figure 1 (left and middle), the ABP will follow a persistent trajectory with persistence time  $\tau_r$  and persistence length  $\xi = v_0 \tau_r$ .

We can interpret the prefactor as follows: When  $\tau_r \to 0$ ,  $\frac{1}{\tau_r}e^{-|t-t'|/\tau_r} \to \delta(t-t')$ , and we recover thermal noise, but with effective diffusion constant  $\frac{v_0^2\tau_r}{2}$ . This system will then carry out a normal diffusive motion without the active persistent part.

In general, this equation gives us an effective active diffusion constant

$$D_a = \frac{v_0^2 \tau_r}{2} \equiv \frac{k_b T_{\text{eff}}^{\text{act}}}{\zeta} \tag{31}$$

Here in the last step we have defined the **effective active temperature** as the temperature we would get if we **pretend that fluctuation-dissipation holds**. This method, which looks at first glance like cheating, is one of the standard ways of defining an effective temperature for an out of equilibrium system.

We can more clearly see what this means for our ABP by computing the mean-square displacement  $MSD(t) = \langle | \boldsymbol{r}(t) - \boldsymbol{r}(0) |^2 \rangle$ . After a pretty lengthy calculation that is similar to the thermal calculation of the MSD, one derives

$$MSD(t) = 4D_t t + 2v_0^2 \tau_r \left[ t - \tau_r (1 - e^{-t/\tau_r}) \right].$$
 (32)

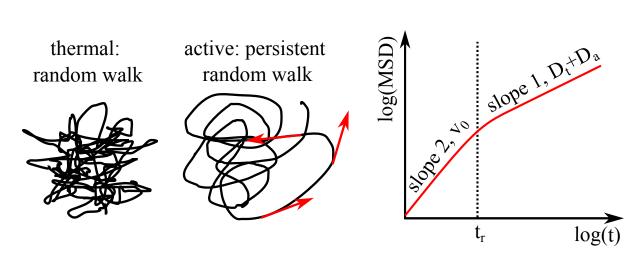


Figure 1: Active Brownian motion: Left - Thermal random walk trajectory. Middle: Active trajectory, persistent random walk. Right: Mean-square displacement for an active Brownian particle.

This function is plotted in 1 (right) in log-log scales.

The first term in this equation is simply normal thermal diffusion with diffusion constant  $D_t$ . We have the two following limits:

• For  $t \ll \tau_r$ : If we set  $D_t = 0$ , like is often down in simulations, the second term describes the active motion only, and we have

$$MSD(t) = v_0^2 t^2. (33)$$

This is the **ballistic motion** where the particle goes at speed  $v_0$  in a straight line, so  $x(t) \approx v_0 t$ .

• For  $t \ll \tau_r$ , we find

$$MSD(t) = 4[D_t + D_a]t, (34)$$

where  $D_a = \frac{v_0^2 \tau_r}{2}$  is the effective active diffusion constant we introduced above. You can now see that the particle at long times diffusions like a normal colloid, but with a new, larger effective diffusion coefficient  $D_{\text{eff}} = D_t + D_a$ . Mapping this then to an effective fluctuation-dissipation result then explains why we would like to introduce an effective temperature  $\frac{v_0^2 \tau_r}{2} \equiv \frac{k_b T_{\text{eff}}^{\text{act}}}{\zeta}$ .

Hydrodynamic models of active materials

#### 3.2 Symmetries

In last week's lecture and exercise, we studied the dynamics of microscopic active materials, such as Active Brownian particles. In the exercise session, we also briefly added alignment to the model. We generically derived the Langevin equations of motion for a particle self-propelled with velocity  $v_0$  along direction  $\mathbf{n} = (\cos \theta, \sin \theta)$ 

$$\dot{\mathbf{r}}_i = v_0 \hat{n}_i + \mu \sum_{ij} \mathbf{F}_{ij} + \boldsymbol{\eta}_i \tag{35}$$

$$\dot{\theta}_i = \mu_r \sum_{ij} T_{ij} + \eta_i^r, \tag{36}$$

where  $\mu = 1/\zeta$  is a mobility (inverse friction) coefficient, and  $\mu_r = 1/\zeta_r$  is a rotational mobility (inverse rotational friction) coefficient. The two noises are for the spatial part  $\langle \boldsymbol{\eta}_i(t) \cdot \boldsymbol{\eta}_j(t') \rangle = 2D\delta_{ij}\delta(t-t')$  and  $\langle \boldsymbol{\eta}_i^r(t) \boldsymbol{\eta}_j^r(t') \rangle = 2D_r\delta_{ij}\delta(t-t')$  where D is a translational and  $D_r$  is a rotational diffusion constant. We can, but don't have to, choose them to follow equilibrium fluctuation-dissipation relations  $D = dk_b T/\zeta$  and  $D_r = k_b T/\zeta_r$ .

The pair forces  $\mathbf{F}_{ij}$  come from the mechanical interactions between particles. For example, in the exercise we chose a central potential, one-sided harmonic spring interactions, which is appropriate for round particles. It depends only on the distance between particle,  $|\mathbf{r}_j - \mathbf{r}_i|$ . If our particles were elongated, such as rods, we would have to also take into account the angles  $\theta_i$  and  $\theta_j$  of the particles.

The pair torques  $\mathbf{T}_{ij}$  determine the (deterministic part of) the particle reorientations. For ABPs,  $T_{ij} = 0$ , which makes them a very clean and easy model system. In general, however  $T_{ij} \neq 0$ . This could be either through mechanical pair torques like for interacting rods, or through explicit interactions between the active directions. Consider the rotational interaction potentials

$$V_p(\mathbf{n}_i, \mathbf{n}_j) = -\frac{J}{\mu_r} \mathbf{n}_i \cdot \mathbf{n}_j = -J \cos(\theta_i - \theta_j)$$

$$V_n(\mathbf{n}_i, \mathbf{n}_j) = -\frac{J}{2\mu_r} \left[ (\mathbf{n}_i \cdot \mathbf{n}_j)^2 - |\mathbf{n}_i \times \mathbf{n}_j|^2 \right] = -\frac{J}{2} \cos(2(\theta_i - \theta_j))$$

These then give rise to angular equations of motion  $\dot{\theta}_i = -\mu_r \partial_{\theta_i} V_r + \eta_r$ , specifically

$$\dot{\theta}_i = -J\sin(\theta_i - \theta_j) + \eta_i^r$$

$$\dot{\theta}_i = -J\sin(2(\theta_i - \theta_j)) + \eta_i^r.$$

For both potentials, as long as J > 0, there is a minimum when  $\theta_i = \theta_j$ , and  $\dot{\theta} = 0$ . These are **aligning** interactions, which make the spins (directions of self-propulsion) of different particles align with each other, and we used the first one to generate a flocking simulation last week. The second interaction is also aligning, but in addition there is a potential minimum at  $\theta_i - \theta_j = \pm \pi$ , i.e. when the spins are **anti-aligned**. In practice, this means that configurations of spins that either point parallel or anti-parallel are both

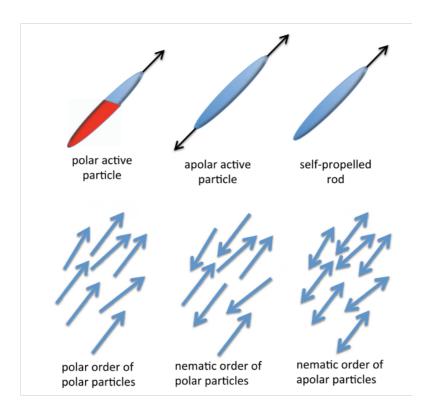


Figure 2: A partial list of symmetries for active particles, image taken from [1].

favoured. In contrast, for both interactions, spins that are orthogonal  $(\theta_j - \theta_i = \pm \pi/2)$  are a potential maximum and so discouraged. We call the first interaction **polar** and the second interaction **nematic**. The Vicsek model model angle interaction can formally be written as

$$\theta(t + \Delta t)_i = \text{angle}\left[\sum_{j \in R} \hat{n}_j(t)\right] + \eta_r,$$
 (37)

where the sum is over all spins within radius R of the central spin and  $\eta_r$  is a white noise. This is also a **polar** interaction that leads to flocking. In contrast, the (complicated) mechanical pair torques between moving rods are **nematic**, as rods do not have a front and a back end. In general we can have any combination of these symmetries (see Figure 2)

## 3.3 Deriving hydrodynamic equations

In lesson 1, we derived a general Fokker-Planck equation that links the microscopic dynamics of a collection of degrees of freedom **A** with its generic Fokker-Planck equation. This technique fully carries over to active materials, and for example we can derive the Fokker-Planck equation of a single ABP in a potential using the same method as for the Smoluchowski equation:

We identify  $\mathbf{A} = (\mathbf{r}, \theta)$ ,  $\mathbf{V} = (v_0 \mathbf{n} - \mu \nabla_{\mathbf{r}} V(\mathbf{r})), 0$ , and the fluctuation correlation matrix  $\mathbf{B}$  with elements  $B_{\mathbf{r},\mathbf{r}} = D\mathbf{I}$ ,  $B_{\theta,\theta} = D_r$  and  $B_{\mathbf{r},\theta} = B_{\theta,\mathbf{r}} = 0$  and the deterministic

 $L_0 = \frac{\partial}{\partial_{\mathbf{r}}} [(v_0 \hat{n} - \mu \nabla_{\mathbf{r}}(\mathbf{r})) P(\mathbf{r}, \theta, t)],$  ultimately giving the Fokker-Planck equation

$$\partial_t p(\mathbf{r}, \theta, t) = -\nabla_{\mathbf{r}} \left[ (v_0 \hat{n} - \mu \nabla_{\mathbf{r}} (\mathbf{r})) p(\mathbf{r}, \theta, t) \right] + D \nabla_{\mathbf{r}}^2 p(\mathbf{r}, \theta, t) + D_r \partial_{\theta}^2 p(\mathbf{r}, \theta, t). \tag{38}$$

We can now see that this equation couples position degrees of freedom  $\mathbf{r}$  and angular degrees of freedom  $\theta$ , and that it does not simply reduce to an equation for the density  $\rho(\mathbf{r})$  like for the Smoluchowski equation.

At the same time, for interacting particles where there are many more degrees of freedom, the Fokker-Planck probability density  $p_N(\mathbf{r}_1,...,\mathbf{r}_N,\theta_1,...\theta_N)$  depends on **all** degrees of freedom and they are usually coupled. These two properties make it **impossible** to directly work with the Fokker-Planck equations except in very specific, usually trivial, cases.

So what do we do instead? At this point, there are many methods, but ultimately, they all boil down to finding a way to approximate the **one-particle probability density**  $p_1(\mathbf{r}, \theta)$  from the many particle probability density  $p_N(\mathbf{r}_1, ..., \mathbf{r}_N, \theta_1, ...\theta_N)$ . This means integrating over all positions and angles except one, and then approximating any interaction terms:

- 1. A formal way to do this is the BBGKY hierarchy [2], where one writes a series of equations for  $p_1$  as a function of  $p_2$ , then  $p_2$  as a function of  $p_3$  and so on. There are then self-consistent methods to cut off the series and approximate interaction terms, for example  $p_2(\mathbf{r}_1, \mathbf{r}_2, \theta_1, \theta_1) \approx (p_1(\mathbf{r}, \theta))^2$ . In general, the BBGKY method, while formally neat, is extremely hard to carry out and not easy to interpret physically. The approximations will also break down for systems that are strongly interacting, e.g. for the dense materials which we have already seen.
- 2. Another formal way to carry this out is a equation using the Boltzmann equation that approximates collisions between a particle and other particles, averaging over all collisions, and so we write an equation for  $p(\mathbf{r}, \theta, t)$  directly. Generically, this can be written as

$$\frac{\partial p(\mathbf{r}, \theta, t)}{\partial t} + \nabla (\mathbf{v}p(\mathbf{r}, \theta, t)) = I_{\text{diff}}[p(\mathbf{r}, \theta, t)] + I_{\text{coll}}[p(\mathbf{r}, \theta, t)], \tag{39}$$

where  $I_{\rm coll}$  are the terms dealing with collisions and  $I_{\rm diff}$  is the diffusion between events - similar to the Fokker-Planck term deriving from noise. The kinetic Boltzmann equation approach has successfully been used to derive equations for the Vicsek model [3]. It is a long and complex calculation, but most of the approximations have already been introduced in the first equation. Again, since it only considers binary collision, we can only use it in the low-density limit.

3. A less formal but very useful and popular approach to writing down these equations is based on symmetries and conservation laws. This has the advantage that it is valid also beyond the low-density limit. However, any parameters of the equation are purely phenomenological and have to be fit. We will return to this approach in a bit.

To make progress towards getting something useful from  $p(\mathbf{r}, \theta, t)$ , the next step is to develop **hydrodynamic** variables, that is quantities that are both observable and and

slowly varying at a macroscopic scale [1]. When we investigated the Smoluchowski equation, we already encountered the hydrodynamic **density** 

$$\rho(\mathbf{r},t) = \frac{1}{2\pi} \int_0^{2\pi} p(\mathbf{r},\theta,t) d\theta, \tag{40}$$

i.e. the angle-averaged probability of finding a particle in a certain region. Since (usually) no particles are created or destroyed, there is a **conservation law** associated with the density, and we can always write the density equation as

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} = -\nabla \cdot \mathbf{J},\tag{41}$$

where **J** is the **conserved current** associated to the density. This equation can have a complicated form, but it will always be written as a gradient.

The next hydrodynamic equations are **angular moments** of the one-particle density, and the symmetry of the underlying dynamics discussed in the previous section will determine which of them are appropriate:

For **polar** system of e.g. flocking spins or aligning active brownian particles, we write down the **polarisation**:

$$\mathbf{p} = \frac{1}{\rho(\mathbf{r}, t)} \int_0^{2\pi} \hat{\mathbf{n}} p(\mathbf{r}, \theta, t) d\theta, \tag{42}$$

that is the averaged direction in which spins are locally pointing. This is a good hydrodynamic variable as long as the spin direction is **slowly varying** locally like e.g. in a bird or Vicsek model flock. Polarisation is a **slow variable**, but it is not a **conserved variable** like the density, so there is not a conserved current associated to it. In a similar vein, and more generally, we can also compute the **hydrodynamic velocity** as

$$\mathbf{v} = \frac{1}{\rho(\mathbf{r}, t)} \int_0^{2\pi} \mathbf{v} p(\mathbf{r}, \theta, t) d\theta. \tag{43}$$

For **nematic** systems, we need to introduce a variable with the correct symmetry  $\hat{\mathbf{n}} \to -\hat{\mathbf{n}}$ . We also want this new variable to not mix with either the density or the polarisation. The **nematic tensor** Q fits the bill:

$$\hat{\mathbf{Q}} = \frac{1}{\rho(\mathbf{r}, t)} \int_0^{2\pi} \left( \hat{\mathbf{n}} \otimes \hat{\mathbf{n}} - \frac{1}{d} \mathbf{I} \right) p(\mathbf{r}, \theta, t) d\theta.$$
 (44)

In addition to being, as requested, symmetric under  $\hat{\mathbf{n}} \to -\hat{\mathbf{n}}$ , this tensor is also **symmetric and traceless**.

Systems with higher order symmetry are rare, but have recently proposed for **quartic** (four-fold) and **hexatic** (six-fold) symmetry. Then a similar approach using 4th (6th) rank symmetric traceless tensor can be employed. If we are using a BBGKY-type moment approach, the equation for  $\rho$  will then depend on  $\mathbf{v}$  and  $\mathbf{p}$  or  $\hat{\mathbf{Q}}$  depending on symmetry. The equation for  $\mathbf{p}$  will depend on  $\hat{\mathbf{Q}}$ , which one then approximated for a polar system as either 0 (disordered), or using  $\mathbf{p} \otimes \mathbf{p}$ . For a nematic, one similarly tries to write higher-order terms as a function of  $\rho$  and  $\hat{\mathbf{Q}}$ . This illustrates both the power and the limitations of the hydrodynamic approach.

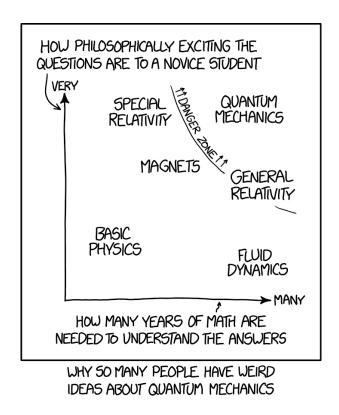


Figure 3: We are in the lower right corner of this image ... Randall Munroe, XCKD [4]

#### 3.4 Hydrodynamics of polar fluids

Let's consider two examples of polar materials: Active Brownian particles without alignment as we have studied already, and a Vicsek model polar flock.

#### MIPS instability

We will begin to illustrate hydrodynamics with a phenomenological model for the motility induced phase separation instability that appears for active Brownian particles (ABPs). Phenomenologically, the reason for the instability is that particles will collide with other particles, which slows them down, with a density dependent velocity that roughly follows  $v(\rho) \approx v_0(1 - \rho/\rho_c)$ . This happens more strongly in regions with high density than low density, and it eventually leads to an overwhelming accumulation of particles in dense region in an instability.

Because ABPs are self-propelled with polar symmetry, despite being disordered, they are still **polar** active matter, but in a disordered phase. We then choose density  $\rho$  and polarisation  $\mathbf{p}(\mathbf{r})$  as hydrodynamic fields. A reasonable phenomenological hydrodynamic model for motility induced phase separation is given by [5]

$$\partial_t \rho = -\nabla \cdot [v(\rho)\mathbf{p} - D(\rho)\nabla \rho] \tag{45}$$

$$\partial_t \mathbf{p} = -D_r \mathbf{p} - \frac{1}{2} \nabla \left[ v(\rho) \rho \right] + K \nabla^2 \mathbf{p}, \tag{46}$$

where  $v(\rho)$  and  $D(\rho)$  are effective particle velocity and effective diffusion,  $D_r$  is the rotational diffusion constant, and K is related to polarisation diffusion.

We can explain this model as follows: We have density conservation in our system, so the right hand side of eq. 45 is still  $\nabla \cdot \mathbf{J}$ , a conserved density current. The next two terms are phenomenological approximations of the angle-coupling terms that we have in the Fokker-Planck equation: We approximate the velocity in the convection term by  $v(\rho)\mathbf{p}$ , i.e. along the polarisation direction with a magnitude  $v(\rho)$  that depends only on the density. The second term is a diffusion term, with an effective diffusion constant  $D(\rho)$ .

The polarisation equation can be read as follows: The first term is the decay of polarisation with rotational diffusion of the particles. The second term resembles the gradient of a pressure, and is proportional the amount of momentum the particles have locally. Finally, the last term is a polarisation diffusion term that with origins in the two diffusion terms of the Fokker-Planck equation.

We can see that this equation does MIPS in a very simple way: If we are in steady-state  $\partial_t \mathbf{p} = 0$ . Then if we also neglect the  $K\nabla^2 \mathbf{p}$  term, we can solve the second equation and write  $\mathbf{p} \approx \frac{1}{2D_r} \nabla[v(\rho)\rho]$ . Back in the first equation, this can be written as

$$\begin{split} \partial_t \rho &= + \boldsymbol{\nabla} \cdot \left[ \frac{v(\rho)}{2D_r} \boldsymbol{\nabla} [v(\rho)\rho] + D(\rho) \boldsymbol{\nabla} \rho \right] \\ &= \boldsymbol{\nabla} \cdot \left[ \left( \frac{v^2(\rho)}{2D_r} + \frac{v(\rho)}{2D_r} \frac{dv(\rho)}{d\rho} + D(\rho) \right) \boldsymbol{\nabla} \rho \right] \\ &= \boldsymbol{\nabla} \cdot \left[ \left( \frac{v^2(\rho)}{2D_r} \left\{ 1 + \frac{d \ln v(\rho)}{d \ln \rho} \right\} + D(\rho) \right) \boldsymbol{\nabla} \rho \right] \\ &= \boldsymbol{\nabla} \cdot [D_{\text{eff}}(\rho) \boldsymbol{\nabla} \rho] \end{split}$$

Here we have rewritten the density equation and an effective diffusion equation, with diffusion coefficient  $D_{\rm eff}(\rho) = D(\rho) + \frac{v^2(\rho)}{2D_r} \left\{ 1 + \frac{d \ln v(\rho)}{d \ln \rho} \right\}$ . As we know, a diffusion equation smoothen out density fluctuations - that is, as long as  $D_{\rm eff}(\rho) > 0$ . What happens here is that since  $v(\rho)$  is a decreasing function of  $\rho$ ,  $\frac{d \ln v(\rho)}{d \rho} < 0$ , and there comes a point when  $D_{\rm eff}(\rho) \leq 0$ . This is the MIPS instability, where density fluctuations will be be amplified instead of of decaying! Further reading: A good MIPS review paper with different derivation of the instability from run-and-tumble dynamics is Tailleur & Cates (2015) [6].

#### Polar or Toner-Tu flocking equations

These equations for the Vicsek model and related polar flocking models of point particles were first derived by John Toner and Yuhai Tu in 1998 [7]. They were originally entirely based on symmetry arguments. The derivation here uses a free energy functional approach and is based on the treatment by Marchetti et al. in [1].

Density is conserved in this model. Therefore, we again write a continuity equation, and

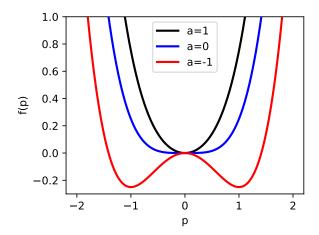


Figure 4: Landau free energy part for **p** from the Toner-Tu equation free energy.

a separate equation for the polarisation

$$\frac{d\rho}{dt} = -\nabla \cdot \mathbf{J}$$

$$= -v_0 \nabla \cdot (\rho \mathbf{p}) - \nabla \left( -\frac{1}{\gamma_p} \nabla \frac{\delta F_p}{\delta \rho} + \mathbf{f}_\rho \right)$$

$$\frac{\partial \mathbf{p}}{\partial t} + \lambda_1 (\mathbf{p} \cdot \nabla) \mathbf{p} = -\frac{1}{\gamma} \frac{\delta F_p}{\delta \mathbf{p}} + \mathbf{f}$$
(48)

In the first equation, the first term is the same convective flux  $\rho \mathbf{v}$  as in the MIPS equation. In the second term, we have what is called Model B dynamics for a conserved variable in overdamped dynamics where we approximate the current J to derive from a free energy (compare to the  $\partial_x^2 V$  term in the Smoluchowski equation). We have also added a purely phenomenological white noise term  $\mathbf{f}_{\rho}$ 

In the second equation, the  $\lambda_1(\mathbf{p} \cdot \nabla)\mathbf{p}$  term is convection of the polarisation field. On the second side, we have what is called model A dynamics for a non-conserved variable, equivalent to plain overdamped relaxation towards the value  $\frac{\delta F_p}{\delta \mathbf{p}}$  given by the free energy. For more information on this topic, please see the 'hydrodynamics' chapter of Chaikin & Lubensky [8].

The free energy here is phenomenological, i.e. it is specifically constructed to give us the result that we want, a flocking transition:

$$F_p = \int d\mathbf{r} \left\{ \frac{\tilde{\alpha}}{2} |\mathbf{p}|^2 + \frac{\tilde{\beta}}{4} |\mathbf{p}|^4 + \frac{\tilde{K}}{2} |\nabla \mathbf{p}|^2 + \frac{w}{2} |\mathbf{p}|^2 \nabla \cdot \mathbf{p} - w_1 \nabla \cdot \mathbf{p} \frac{\delta \rho}{\rho_0} + \frac{A}{2} \left( \frac{\delta \rho}{\rho_0} \right)^2 \right\}$$
(49)

The density part is simply quadratic with  $\delta\rho$  being density fluctuations around a mean density  $\rho_0$ . That is designed to create a pretty straightforward convection and diffusion density equation  $\frac{d\rho}{dt} + v_0 \nabla \cdot (\rho \mathbf{p}) = \nabla \cdot \left(\frac{A}{\gamma_p} \nabla \delta \rho + \mathbf{f}_\rho\right)$ . The polarisation piece includes in its first three terms a Landau-type free energy with a transition as a function of the sign

of  $\tilde{\alpha}$ :

$$f_{\text{Landau}}(\mathbf{p}) = \frac{\tilde{\alpha}}{2} |\mathbf{p}|^2 + \frac{\tilde{\beta}}{4} |\mathbf{p}|^4 + \frac{\tilde{K}}{2} |\nabla \mathbf{p}|^2$$
 (50)

As shown in Figure 4, at the mean field level this is the classic potential from field theory and magnetism which has a single minimum at  $\mathbf{p} = 0$  for  $\tilde{\alpha} > 0$ , and then develops a whole ring of solutions with  $|\mathbf{p}| = \sqrt{\frac{-\tilde{\alpha}}{\tilde{\beta}}}$ . This means that, in the absence of an external field, the system randomly selects a polarisation vector  $\mathbf{p}$  through spontaneous symmetry breaking. This is the flocking transition, and at the mean field level, it works just like the Landau mean field theory of magnetisation - though note that just like in magnetism, mean field here is not accurate either.

The remaining terms in the free energy are then dictated by symmetry, and consist of all the other terms to combined second order in  $\boldsymbol{p}$  and  $\delta\rho$  that are compatible with creating a scalar. We neglect all higher order terms. Finally, the Toner-Tu equations are given by

$$\partial_t \boldsymbol{p} + \lambda_1 (\boldsymbol{p} \cdot \boldsymbol{\nabla}) \boldsymbol{p} = -\left[\alpha(\rho) + \beta |\boldsymbol{p}|^2\right] \boldsymbol{p} + K \nabla^2 \boldsymbol{p} - \nu_1 \boldsymbol{\nabla} \frac{\rho}{\rho_0} + \frac{\lambda}{2} \boldsymbol{\nabla} |\boldsymbol{p}|^2 - \lambda \boldsymbol{p} (\boldsymbol{\nabla} \cdot \boldsymbol{p}) + \mathbf{f}$$
(51)

It is instructive at this point to briefly compare this equation to the Navier-Stokes equation for a fluid with velocity  $\mathbf{v}$ :

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \mathbf{v}, \tag{52}$$

where P is the pressure and  $\nu$  is the viscosity.

The structure of the equation has similarities to the polarisation, but also strong differences: The Navier-Stokes equation derives from a conservation law, momentum conservation, i.e. ultimately Newton's law again. This has two consequences: first,  $\lambda_1 = 1$  by necessity, and this convective term is usually derived by introducing a Eulerian (absolute) frame from a Lagrangian (material) frame. Second, the right-hand side is  $\nabla \cdot \hat{\boldsymbol{\sigma}}$ , where  $\hat{\boldsymbol{\sigma}}$  is the stress tensor of the fluid, and it can only include gradient terms due to this. In contrast, the Toner-Tu polarisation equation has linear and quadratic terms in  $\boldsymbol{p}$ .

From this one can develop the transition line in the model in mean-field by setting all gradients to zero.

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