Stability of a 2D active fluid on a substrate

2017-2018 Statistical Mechanics exam – iCFP M2 – Soft Matter & Biophysics track

Beyond the study of usual equilibrium fluids, solutions of self-driven particles—so-called "active fluids"—have attracted much interest in recent years. In the most common experimental geometry, a thin two-dimensional layer of an aqueous solution containing, *e.g.*, bacteria or components of the cell's cytoskeleton are deposited onto a substrate. These particles are typically not spherically symmetric, and display local nematic alignment. When provided with the suitable fuel however, the uniform, motionless nematic state can become unstable, giving rise to spontaneous flow in the system.

In most of this exercise, we develop a phenomenological theory that accounts for the stability of these two-dimensional fluids, which we characterize by their local orientation field $\theta(\mathbf{r})$ in the (x, y) plane as well as their (two-dimensional) momentum density $\mathbf{g}(\mathbf{r})$. Here $\mathbf{r}$ is a two-dimensional position vector. While mass and the number of bacteria are typically conserved in experimental realizations of these fluids, here we do not include these variables in our description for simplicity. We will consider an isothermal system throughout.

Section 1 builds a simple phenomenological theory for the basic case of an equilibrium fluid only characterized by an orientational field. Section 2 does the same for an equilibrium fluid with only $\mathbf{g}(\mathbf{r})$. Section 3 then couples the two aspects at equilibrium, and Sec. 4 tackles the active, nonequilibrium case. While these sections are strongly related with one another, any section can in principle be tackled independently from the preceding ones. Finally, Sec. 5 proposes an independent and largely unrelated free-form exercise; while little guidance is provided in the text, taking it to completion with a convincing discussion will be well rewarded.

1 Phenomenological dynamics of a two-dimensional nematic

Here we consider a medium composed of nematic particles and describe it solely through its orientational field $\theta(\mathbf{r})$.

1.1 We first derive the medium's free energy functional from a microscopic picture. We consider a collection of two-dimensional XY spins with orientation $\mathbf{S}_i = (\cos\theta_i, \sin\theta_i)$ residing on a two-dimensional square lattice with lattice spacing equal to a and governed by a free energy function identical to the Hamiltonian of the XY model:

$$F = -\tilde{K} \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{1}$$

Taking the $a \to 0$ continuum limit of F in the spin-wave regime, show that over large length scales the system is governed by the Franck free energy in the one-constant approximation, namely

$$F = \int \frac{K}{2} (\nabla\theta)^2 \, \mathrm{d}\mathbf{r}, \tag{2}$$

where you will express K as a function of $\tilde{K}$ and a.

1.2 Under what transformations of the coordinate system and order parameter is this continuum system invariant? For each transformation considered specify how $\mathbf{r}$, ∇ and θ are transformed. Specify the parity of the order parameter under time reversal.

1.3 Write the most generic phenomenological dynamics for $\theta(\mathbf{r}, t)$ as a function of a derivative of the free energy. We will not invoke any conservation equation here or in the following sections. You can denote the kinetic coefficient involved by $\gamma^{\theta\theta}$.

1.4 Establish that the evolution equation for the system reads

$$\partial_t \theta = D \Delta \theta \tag{3}$$

and relate the new coefficient D to K. What is the sign of D and why (detailed proof not required)?

2 Phenomenological dynamics of a fluid on a substrate

We now consider a fluid described solely by its linear momentum density $g(\mathbf{r})$, and neglect the fact that its mass density is conserved. This is equivalent to assuming an infinitely compressible fluid, a system in contact with a particle reservoir in every point or the type of Malthusian flocks discussed in our lectures.

2.1 Enumerate the symmetries of the system and the order parameter as in the previous section.

2.2 Specify its free energy functional.

2.3 Write the system's phenomenological dynamics as in question 1.3. Do not take advantage of symmetries yet.

2.4 Show that if for any rotation matrix l we have $l_{ij}\gamma_{jk} = \gamma_{ij} l_{jk}$, then the rank two tensor γ must be of the form

$$\gamma = \begin{pmatrix} \gamma_{11} & \gamma_{12} \\ -\gamma_{12} & \gamma_{11} \end{pmatrix} \tag{4}$$

2.5 Enforce a rotational symmetry to be specified on your evolution equation, and formulate an evolution equation with two unknown kinetic coefficients.

2.6 Using an additional symmetry to be specified, show that the evolution equation reads

$$\partial_t g_i = -\gamma^{gg} v_i \tag{5}$$

2.7 What is the physical meaning of v_i? What about γ^{gg}? What is the sign of γ^{gg} and why?

2.8 Is $\mathbf{g}$ a conserved quantity in this system? Why? How should you change the system to make it into one?

3 Nematic fluid on a substrate at equilibrium

We now couple the dynamics of the broken symmetry variable $\theta(\mathbf{r})$ and the non-conserved order parameter $g(\mathbf{r})$ at equilibrium, keeping in mind that their separate evolutions are described by Eqs. (3) and (5).

3.1 Write the coupled phenomenological dynamics to zeroth order in gradients as a linear relationship between the time derivatives of $\theta(\mathbf{r})$ and $g(\mathbf{r})$ on the one hand, and the functional derivatives $\frac{\delta F}{\delta \theta(\mathbf{r})}$ and $\frac{\delta F}{\delta g_i(\mathbf{r})}$ on the other. This introduces two sets of new kinetic coefficients.

3.2 Are the couplings corresponding to these coefficients reactive or dissipative? Why?

3.3 There is a relationship between the two sets of new coefficients. What is it called and what form does it take here (no proof required)? Under what condition is this relationship valid?

3.4 Use a symmetry of the system to prove that the newly introduced kinetic coefficients are actually equal to zero.

3.5 As a consequence of this, we will use an expansion in powers of the gradient of the thermodynamic forces $\frac{\delta F}{\delta \theta(\mathbf{r})}$ and $\frac{\delta F}{\delta g_i(\mathbf{r})}$. What is the physical meaning of such an expansion?

3.6 Write these gradient couplings in their most general form, introducing two tensors of kinetic coefficients $\gamma_{ij}^{\theta g}$ and $\gamma_{ij}^{g\theta}$.

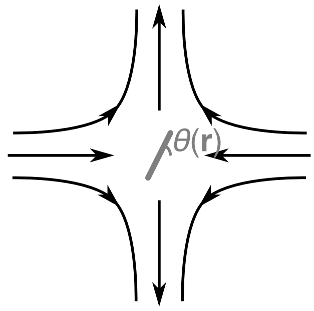

Figure 1: A nematic particle (grey) aligning in an extensional flow whose flow lines are pictured in black.

3.7 What is now the relationship between these two new tensors (see next question if you cannot remember)?

3.8 We now work to prove this relationship in this question and the next. First establish a relationship between the correlators $\langle \theta(\mathbf{r},t) g_i(\mathbf{r}',0)\rangle$ and $\langle \theta(\mathbf{r},0) g_i(\mathbf{r}',t)\rangle$ for a system with time-reversible microscopic dynamics.

3.9 Now use this result to prove the relation of question 3.7, remembering that at equilibrium

$$\left\langle a(\mathbf{r}) \frac{\delta F}{\delta a(\mathbf{r}')} \right\rangle = \delta(\mathbf{r}-\mathbf{r}'). \tag{6}$$

For simplicity, you may set $\gamma^{\theta\theta} = 0$ and $\gamma^{gg} = 0$ to answer this question.

3.10 We now endeavor to determine the form of the coupling between $\partial_t \theta$ and $\partial_i \frac{\delta F}{\delta g_j(\mathbf{r})}$. First, state how all variables entering your evolution equations transform under a mirror symmetry with respect to the horizontal x axis.

3.11 Next, exploit this symmetry to show that the diagonal entries of the tensor of couplings introduced in this section vanish.

3.12 To determine one more phenomenological coefficient, we impose the minimal requirement that the θ-equation must be compatible with a homogeneous nematic fluid that rotates with a constant angular rate Ω around the origin of coordinates. What is the expression of the velocity field in such a fluid? How about the θ field?

3.13 Insert these expressions in the θ equation to find one more constraint on the remaining kinetic coefficients. Write the most general form of the remaining evolution equations, where the coupling between θ and $\mathbf{v}$ now involves only one unknown coefficient.

Physically, the remaining parameter describes whether the particles tend to align their director with the x or y axis in the flow geometry schematized in Fig. 1, as well as the strength of this flow coupling. In the following we take the particular case where no such alignment with the flow takes place and use the following simplified equations of motion:

$$\partial_t \theta = D\Delta\theta + \frac{1}{2}\partial_x v_y - \frac{1}{2}\partial_y v_x \tag{7a}$$

$$\partial_t g_x = \frac{1}{2}\partial_y \Delta\theta - \gamma^{gg} v_x \tag{7b}$$

$$\partial_t g_y = -\frac{1}{2}\partial_x \Delta\theta - \gamma^{gg} v_y. \tag{7c}$$

4 Active orientable fluid on a substrate

In Eqs. (7) (just before), the cross-couplings between θ and g_i are constrained due to Onsager symmetry. We now consider an active system, where no such constraint exist. To reflect this, we introduce a so-called "active force" $\mathbf{f}(\theta, \nabla\theta, ...)$, thus adding two terms f_x and f_y to the right-hand-sides of Eqs. (7b) and (7c) respectively. The resulting couplings of $\mathbf{g}$ to θ have no counterpart in Eq. (7a), and that fact violates Onsager symmetry. In the following we consider only small perturbations about a nematic state aligned along the x axis (*i.e.*, states where θ is a small quantity)

4.1 What is the most general form of $\mathbf{f}$, not taking symmetries into account for now?

4.2 Use symmetries to show that $\mathbf{f}$ vanishes in the fully ordered state $\theta(\mathbf{r}) = 0$, and depends on θ only through its gradients.

4.3 Use an additional symmetry (possibly inspired by Sec. 3) to show that

$$f_x = -(\zeta_1 + \zeta_2)\partial_y\theta \tag{8a}$$
$$f_y = -(\zeta_1 - \zeta_2)\partial_x\theta. \tag{8b}$$

4.4 Write the full equations of motion for the active system. Assuming that the system is overdamped (*i.e.*, that its inertia is negligible), eliminate $\mathbf{v}$ and expand to lowest order in gradients to find

$$\partial_t\theta = \tilde{D}\Delta\theta + \frac{\zeta_1}{2\gamma^{gg}}\left(\partial_y^2\theta - \partial_x^2\theta\right) \tag{9}$$

and specify the expression of $\tilde{D}$.

4.5 To assess the stability of the system, we consider a small perturbation to it that has the form of a plane wave:

$$\theta(\mathbf{r}) = \theta_0(t)e^{i\mathbf{q}\cdot\mathbf{r}} \tag{10}$$

with $\mathbf{q} = q(\cos\phi\hat{\mathbf{x}} + \sin\phi\hat{\mathbf{y}})$. Solve the evolution equation for $\theta_0(t)$.

4.6 Since any perturbation can be decomposed into a superposition of plane waves, the system is guaranteed to be stable only if all possible plane waves (*i.e.*, plane waves with all possible values of q and ϕ) are stable. Use this insight to construct a phase diagram for the system as a function of parameters $\zeta_1/\gamma^{gg}D$ and $\zeta_2/\gamma^{gg}D$, distinguishing between the stable and unstable regions.

5 Colored noise in the Langevin equation

We consider an Ornstein-Uhlenbeck process with so-called colored noise:

$$\partial_t x(t) = -x(t) + \xi(t) + f(t) \tag{11}$$

with ξ a Gaussian noise satisfying $\langle\xi(t)\rangle = 0$ and $\langle\xi(t)\xi(t')\rangle = \lambda e^{-\lambda|t|}$ and $f(t)$ an externally applied force. Show that even in the stationary regime this process does not satisfy the fluctuation-dissipation relation in Fourier space

$$\tilde{\chi}''(\omega) = \frac{\omega\tilde{C}(\omega)}{2}, \tag{12}$$

where the Fourier transform is defined by $\tilde{f}(\omega) = \int_{-\infty}^{\infty} f(t)e^{i\omega t}\,dt$. Why not? In what limit is the fluctuation-dissipation relation satisfied? Why? The relevance and clarity of your discussion will be especially valued in this section.