Arnold Sommerfeld Center for Theoretical Physics
LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN
Winter Term 2025

Prof. Erwin Frey
A. Winter, D. Toffenetti,
N. Dominko Kobilica,
K. Wharam

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# Self-organization and pattern formation
# Sheet 6

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## Exercise 17 – Linear Stability of the Keller–Segel Model

Consider the Keller–Segel model for chemotaxis, which you have seen in the lecture. This model describes a coarse-grained density of living cells which produce a chemical they are themselves attracted towards (a *chemoattractant*). The chemoattractant can decay over time, but the total number of cells is assumed to be constant. Both the cells (density $\rho(x,t)$) and the chemical (concentration $c(x,t)$) can diffuse in space, with diffusion constants $D$ and $D_c$ respectively, leading to the following set of equations:

$$\frac{\partial \rho(x,t)}{\partial t} = D\nabla\left(\nabla\rho(x,t) - \chi(c)\rho(x,t)\nabla c(x,t)\right)\,, \tag{1}$$

$$\frac{\partial c(x,t)}{\partial t} = \alpha(\rho) - \lambda c(x,t) + D_c\nabla^2 c(x,t)\,, \tag{2}$$

where $\chi(c)$ describes the chemotactic sensitivity, $\alpha(\rho)$ is the chemoattractant production rate and $\lambda$ is the chemoattractant decay rate. In contrast to what you have already seen in the lecture, we want to discuss different sensitivity and production models in this exercise. Thus, we set

$$\chi(c) = \frac{\chi_0}{1 + c/\tilde{c}}\,, \qquad \alpha(\rho) = \alpha_0\frac{\rho}{1+\beta\rho}\,. \tag{3}$$

**a)** Explain the structure of the terms $\chi(c)$ and $\alpha(\rho)$ and the meaning of all constants. Why are these terms sensible assumptions in biological systems?

**b)** Show that the system admits a spatially homogeneous steady state

$$\rho(x,t) = \rho_0, \qquad c(x,t) = c_0\,, \tag{4}$$

and calculate the relation that has to hold between $\rho_0$ and $c_0$.

**c)** Perform a linear stability analysis of the homogeneous steady state. For simplicity we assume $\tilde{c} = c_0$ for all following exercise parts. Consider small perturbations:

$$\rho(x,t) = \rho_0 + \delta\rho(x,t), \qquad c(x,t) = c_0 + \delta c(x,t), \tag{5}$$

and linearize the equations to first order in $\delta\rho$ and $\delta c$.

**d)**
Assume solutions of the form

$$\delta\rho(x,t) \sim e^{\sigma t}e^{ikx}\,,\; \delta c(x,t) \sim e^{\sigma t}e^{ikx} \tag{6}$$

and derive the dispersion relation $\sigma(k)$.

**e)** Determine the condition under which the homogeneous state becomes linearly unstable. That is, find the values of $\rho_0$ and $\chi_0$ (in terms of other parameters) for which $\mathrm{Re}(\sigma(k)) > 0$ for some $k \neq 0$. Plot and interpret your dispersion relation.

**f)** Discuss the physical interpretation of this instability in terms of chemotactic aggregation. And compare this result to a linear production and sensitivity (see lecture notes).

# Exercise 18 – Active Model B and Pseudopotentials

*Note that this exercise counts as two exercises (2P) since it is quite lenghty.*

Active matter equations contain terms which cannot be obtained minimizing any free energy, as the system is dissipating energy. The consequence is that a stationary state in active matter does not correspond to some minimum of a free energy, and finding its explicit form can be challenging.

However, it is sometimes possible to introduce pseuso-thermodynamical variables, which allows us to use the well-known tools for the thermodynamical case despite the lack of any physical correspondance. In this exercise, you will see how to introduce pseudo-variables for active model B and active model B+ and calculate the value of the binodal densities for active model B+.

We consider a density $\phi$ that follows the dynamics of active model B+. The dynamic equation for $\phi$ consist of an equilibrium flux derived from a free energy functional $\mathcal{F}$ and an additional active contribution

$$\partial_t\phi = -\nabla\cdot J\,, \tag{7}$$

$$J = -\nabla[\frac{\delta\mathcal{F}}{\delta\phi} + \lambda(\nabla\phi)^2] + \xi(\nabla^2\phi)\nabla\phi\,, \tag{8}$$

$$\mathcal{F} = \int d^dx\, f(\phi) + \frac{K}{2}(\nabla\phi)^2. \tag{9}$$

**a)** How are the equations for active model B (AMB) and passive model B related to active model B+ (AMB+) (in D-dimensions)?

**b)** Argue why the current in active model B+ cannot be written in terms of a total derivative for dimension greater than one. Argue how this allows for the existence of active currents in the steady state. How are the equations for active model B and active model B+ related in 1D?

First, we consider a phase separated system into a low $\phi(\infty) = \phi_-$ and high density $\phi(-\infty) = \phi_+$ phase with a flat interface so we can consider the 1-dimensional equations.

**c)** We start by revisiting the tools for the passive phase separating system so we can later apply this to our active system. For a passive system showing phase separation (passive model B), the two thermodynamical variables that have to remain constant across a stationary interface are the pressure $P = \mu\phi - f(\phi)$, ensuring mechanical equilibrium, and the chemical potential $\mu$, ensuring that there is no particle flux across the interface. Show that in 1D (flat interface) these two variable are constant in passive model B.

*Hint: To show that the pressure is constant, multiply the chemical potential* $\mu = \frac{\delta F}{\delta \phi}$ *by* $\partial_x \phi$ *and then integrate it over space.*

**d)** Show that the nonequilibrium chemical potential

$$\mu_{\text{neq}}^{\text{AMB}} = \frac{\delta \mathcal{F}}{\delta \phi} + \lambda (\nabla \phi)^2 \tag{10}$$

also remains constant across a stationary and flat interface in active model B (AMB) (1D), while the pressure $P$ is not constant.

**e)** To generalize the concept of mechanical equilibrium in active model B, we introduce a pseudo-density $\psi$ and pseudo-potential $g(\psi)$ which obey the following relations:

$$\frac{df(\phi)}{d\phi} = \frac{dg(\psi)}{d\psi}, \qquad K\partial_\phi^2 \psi = -2\lambda \partial_\phi \psi \tag{11}$$

Show that with this change of variables, the pseudo-pressure $\tilde{P} = \mu\psi - g(\psi)$ is constant across the interface.

*Hint: Show first that*

$$\partial_x \psi \left( K \partial_x^2 \phi - \lambda (\partial_x \phi)^2 \right) = \partial_x \left( \frac{K \partial_\phi \psi}{2} (\partial_x \phi)^2 \right). \tag{12}$$

*Then multiply equation 10 by* $\partial_x \psi$ *and then integrate it over space as you did in part a).*

**f)** Use your result from (b) and (e) to define the relations for the pseudopotential for active model B+ in 1D.

**g)** * *This exercise is voluntary but demonstrates the idea nicely.**
We want to use the derived conditions for the pseudopotential and the nonequilibrium chemical potential to numerically determine the binodals for active model B+. We assume that the free energy functional is given by

$$F[\phi] = \int \mathrm{d}^d x \left( -\frac{A}{2}\phi^2 + \frac{A}{4}\phi^4 + \frac{K}{2}(\nabla \phi)^2 \right), \tag{13}$$

with $A = \frac{1}{4}$ and $K = 1$.

Determine the values for $\phi_\pm$ following the provided mathematica notebook.

In the last parts of this exercise we consider a curved interface and calculate the corrections to the previously derived condition for the pseudopotential for active model B+ (Remember the Laplace pressure for a curved interface in passive model B). For this we consider a high density droplet $\phi(r=0)=\phi_+$ of radius $R$ in a low density environment $\phi(r=\infty)=\phi_-$. Remember from exercise (b) that the current in active model B+ can not be written in terms of a total derivative in dimensions greater than one. Thus, deriving the nonequilibrium potential $\mu_{\text{neq}}^{AMB+}$ for dimensions greater than 1 is a little more envolved.

**h)** In order to derive the nonequilibrium chemical potential we use the Helmholtz decomposition of a vector to rewrite the current into a gradient and curl contribution: $J=-\nabla\mu_{\text{neq}}^{\text{AMB+}}+\nabla\times A$. For this, calculate $\mu_{\text{neq}}^{\text{AMB+}}$ for the case of a spherical symmetric droplet. Show that the term proportional to $\xi$ introduces a non-locality into the nonequilibrium chemical potential. Argue why the dynamics of $\phi$ is governed only by the chemical potential $\mu_{\text{neq}}^{AMB+}$ and not by the curl $A$.
*Hint: Interpret the problem in analogy to electrostatics, where the current $J$ is the electric field $E$, $\nabla\cdot E$ the electric charge, while $\mu$ is the electric potential $V$. The corresponding equations of electrostatics are equivalent: $E=-\nabla V$. For a spherically symmetric configuration of the charge, the electric potential $V$ can be calculated as follows*

$$V(r)=-\int_r^\infty dsE(s)\,. \tag{14}$$

*Your result for the chemical potential should read*

$$\mu_{\text{neq}}^{\text{AMB+}}(r)=\frac{\delta F}{\delta\phi}+(\lambda-\frac{\xi}{2})(\nabla\phi)^2+\xi(d-1)\int_r^\infty dr'\frac{(\partial_{r'}\phi(r'))^2}{r'}\,. \tag{15}$$

**i)** Using the nonequilibrium chemical potential derived in the previous exercise, find the relations that the pseudo-pressure (use the definition of the pseudo-potential derived in (f)) and non-equilibrium chemical potential satisfy at a stationary curved interface.

Your result for the pseudo-pressure relation should read

$$\tilde{P}(\phi_+)=\tilde{P}(\phi_-)+\frac{(d-1)}{R}\sigma_{neq} \tag{16}$$

with the nonequilibrium tension

$$\sigma_{neq}=\frac{K}{\xi-2\lambda}\left(\xi e^{\frac{\xi-2\lambda}{K}\phi(0)}\int_0^\infty dr(\partial_r\phi)^2-2\lambda\int_0^\infty dr(\partial_r\phi)^2e^{\frac{\xi-2\lambda}{K}\phi(r)}\right)\,. \tag{17}$$

*Proceed as follows:*
1) *Similar as in (e): multiply eq. 15 by $\partial_r\psi$ and integrate over the radius. Use spherically symmetric coordinates.*
*Note that the hint from (e) can also be used here when replacing $\lambda\to\lambda-\frac{\xi}{2}$*

$$\partial_r\psi\left(K\partial_r^2\phi-(\lambda-\frac{\xi}{2})(\partial_r\phi)^2\right)=\partial_r\left(\frac{K\partial_\phi\psi}{2}(\partial_r\phi)^2\right)\,. \tag{18}$$

3) *Use a sharp interface approximation*

$$\int_r^\infty ds(\partial_s\phi(s))^2 f(s) \approx \Theta(R-r)f(R)\int_0^\infty ds(\partial_s\phi(s))^2 \tag{19}$$

*where* $\Theta(R-r)$ *is the Heaviside theta.*
*4) Insert the value of* $\psi(\phi)$*, found by solving the equation for the pseudovariables*

$$\psi(\phi) = \frac{K}{\xi - 2\lambda}\exp\left(\frac{\xi-2\lambda}{K}\phi\right). \tag{20}$$

**j)** Can the derived nonequilibrium tension $\sigma_{\text{neq}}$ become negative? What does this imply for the radial dynamics of the droplet?
*Hint: We can use the result known from the equilibrium theory (LSW) and simply replace the equilibrium tension* $\sigma_{eq}$ *with its non-equilibrium value* $\sigma_{neq}$

$$\partial_t R \propto \frac{\sigma_{neq}}{R}\left(\frac{1}{R^*} - \frac{1}{R}\right). \tag{21}$$

Your solutions should be handed in in moodle by **Wednesday, December 3 $^{\text{rd}}$ 2025, 10 am.**