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## Self-organization and pattern formation

### Sheet 3

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### Exercise 9 – Source degradation model

A key aspect of protein pattern formation is *bulk-boundary coupling*. In a cell, the bulk is the cytosol inside the cell, and on its boundary is the cell membrane. In this problem, we consider a lower dimensional conceptual analog of this, where the bulk is a one-dimensional line of length  $h$  and the boundary are its endpoints at  $z = 0$  and  $z = h$ . These endpoints are coupled to the dynamic in the cytosol through boundary conditions at  $z = 0$  and  $z = h$ .

The cytosol (bulk) dynamics is, as is often the case, dominated by diffusion, with diffusion constant  $D_c$ , whereas the membrane is reactive. Proteins bind to the membrane at  $z = 0$  with a rate  $k_{\text{on}}$ , which has units [length/time]. At the other end  $z = h$ , the system is closed.

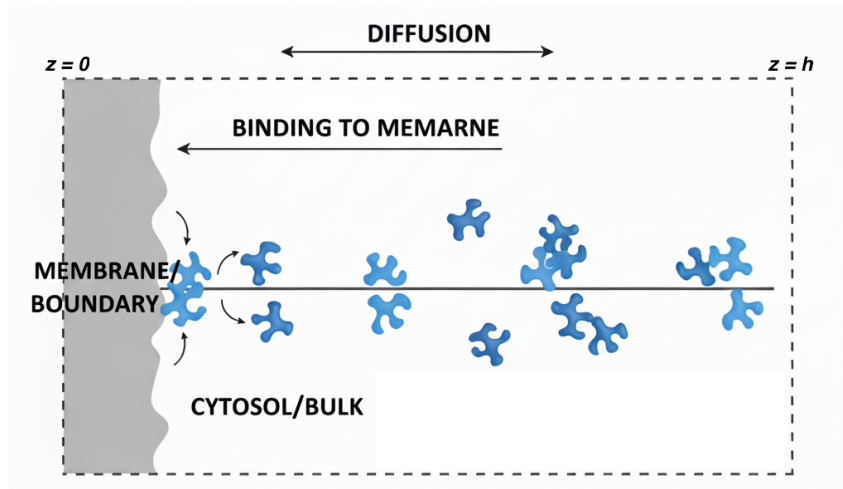


Figure 1: Schematic of the modeled system in Exercise 9.

To model this spatially extended system, we now need to use partial differential equations (PDEs) instead of ordinary differential equations (ODEs). Still, there might be conditions under which we can approximate the bulk density at a certain position by the average (or well-mixed) bulk density, which reduces the system to ODEs again.

In this exercise we will explore under which conditions we are allowed to make this approximation. To this end, we'll start with the fully spatially extended system and derive which conditions need to be fulfilled to allow for an approximation by a well-mixed system. The dynamics of the density of proteins in the bulk is given by the diffusion equation

$$\partial_t c(z, t) = D_c \nabla_z^2 c(z, t). \quad (1)$$

a) Write down the corresponding boundary conditions at  $z = 0$  and at  $z = h$  and give an expression of the dynamics of the membrane bound proteins  $\partial_t m$ .

*Hint: the particle flux  $J(z, t)$  in the bulk is defined by  $\partial_t c(z, t) = -\nabla_z J(z, t)$ .*

b) In case we can neglect the diffusive dynamics in the bulk, we can reduce the diffusion equation to an ODE for the density at  $z = 0$ ,  $\tilde{c}(t) = c(0, t)$ . To this end, define the average bulk density,  $\bar{c}(t)$  and assume  $\tilde{c}(t) \approx \bar{c}(t)$  to arrive at

$$\partial_t \tilde{c}(t) = -\frac{k_{\text{on}}}{h} \tilde{c}(t).$$

Solve this equation. What is the steady state? And what is the relaxation time to arrive at steady state?

c) Since the diffusion equation (1) is analytically solvable, we can also explicitly show under which assumptions the diffusion in the bulk can be neglected. To this end, we want to get an expression for the wavelength of the gradients and compare these to the bulk size  $h$ .

Use the separation ansatz  $c(z, t) = \phi(t)\zeta(z)$  and the separation variable  $\sigma$  to get

$$\partial_t \phi(t) = -\sigma \phi(t) \quad (2)$$

$$D_c \nabla_z^2 \zeta(z) = -\sigma \zeta(z). \quad (3)$$

Use the equation for  $\zeta(z)$  to find the dispersion relation, which is the explicit expression of  $\sigma$  as a function of  $q$ . Find a solution for both  $\phi(t)$  and  $\zeta(z)$  that already satisfies the boundary condition at  $z = h$ .

*Hint: The dispersion relations describe how a frequency  $\sigma$  depends on the wave number  $q$ , i.e. is the function  $\sigma(q)$ . To find it, Fourier transform in the equations both the time (to obtain a frequency  $\sigma$ ) and the space (to obtain a wave number  $q$ ).*

d) Use the boundary condition at  $z = 0$  to derive the eigenvalue condition

$$hq_i \tan(hq_i) = \frac{h}{l_{\text{on}}},$$

with  $l_{\text{on}} = D_c/k_{\text{on}}$ . This equation can only be solved analytically in certain limits. Consider the limits  $h \ll l_{\text{on}}$  and  $h \gg l_{\text{on}}$ . For these limits, find the smallest eigenvalue  $q_1$ , corresponding relaxation time  $\tau_1$  and wavelength  $\lambda_{\text{max}} = \frac{2\pi}{q_1}$ . Compare the relaxation time with the time scale you found in part b).

*Hint: Look at the separation of variables in problem part c) to find an expression of the relaxation time  $\tau_1$  as a function of  $\sigma_1$ .*

e) Use dimensional analysis and the insights gained from the previous problem parts to get an expression for the length scale of the bulk gradients  $l_{\text{on}}$ , the timescale of cytosolic

mixing  $\tau_{\text{diff}}$  and the typical time a protein suspended in the bulk needs to attach to the membrane  $\tau_{\text{on}}$ . Use these quantities to give an argument under which conditions the diffusive dynamics, i.e. gradients, can be neglected.

## Exercise 10 – Allen-Cahn equation with external field

In this exercise, we will examine the behavior of the Allen-Cahn model with an external field in one dimension. The general form of the equation is

$$\partial_t \phi = \kappa \nabla^2 \phi - f'(\phi), \quad (4)$$

where we have set the kinetic coefficient  $\Lambda = 1$  (c.f. lecture) and  $f(\phi)$  is a double-well potential given by Bragg-Williams (mean-field) approximation,

$$f(\phi) = -\frac{r}{2}\phi^2 + \frac{u}{4}\phi^4 - h\phi, \quad (5)$$

with  $h$  an external magnetic field and  $\phi$  corresponds to the magnetization in a magnetic system. Note that this exercise is an extension of the analysis of the Allen-Cahn equation from the lecture notes.

a) Rescale the equation to the form

$$\partial_{\tilde{t}} \tilde{\phi} = \kappa \nabla_{\tilde{x}}^2 \tilde{\phi} - \partial_{\tilde{\phi}} \left[ A(\tilde{\phi} - 1)^2(\tilde{\phi} + 1)^2 - \tilde{h}\tilde{\phi} \right], \quad (6)$$

where  $\tilde{t}$ ,  $\tilde{x}$ ,  $\tilde{\phi}$  and  $\tilde{h}$  are the corresponding rescaled variables to  $t$ ,  $x$ ,  $\phi$  and  $h$ . Use the rescaled form given in the lecture with  $A = \frac{r}{4}\phi_s^2 = \frac{r^2}{4u}$ . Find  $\tilde{h}$ . In the following, rename  $\tilde{t} \rightarrow t$ ,  $\tilde{x} \rightarrow x$ ,  $\tilde{\phi} \rightarrow \phi$  and  $\tilde{h} \rightarrow h$ .

b) What are the possible fixed points of the spatially uniform system? Solve the fixed-point equation graphically. For fixed field  $h$  and bifurcation-parameter  $r$ , what kind of bifurcation do you observe in the non-rescaled system? At which value  $r_c$  does it occur? Draw a bifurcation diagram.

c) Recall the linear stability analysis from the lecture, with the dispersion relation

$$\sigma(q) = -\kappa q^2 - f''(\phi^*). \quad (7)$$

Calculate  $f''(\phi)$  and discuss your result.

d) We will now calculate the front velocity for an interface connecting  $\varphi = \phi_+$  (the higher fixed point in the homogeneous system) at  $x \rightarrow -\infty$  with  $\varphi = \phi_-$  (the lower fixed point in the homogeneous system) at  $x \rightarrow \infty$  for small values of the field  $h$ , which we will choose  $h > 0$  in the following. In order to do so, rewrite Eq. (6) in the co-moving frame such that  $\phi(x, t) = \varphi(z - \zeta(t))$  and show that

$$\partial_t \zeta(t) = \kappa \frac{\Delta f}{\gamma}, \quad (8)$$

where  $\Delta f = f(\phi_-) - f(\phi_+)$  and  $\gamma = \kappa \int_{-\infty}^{\infty} (\partial_z \phi)^2 dz$ . Sketch the interface connecting  $\phi_+$  to  $\phi_-$ . If  $h$  is small, the minima of the potential at  $\phi_{\pm}$  are roughly equal to the values at zero field,  $\phi_{\pm}(h) \approx \phi_{\pm}|_{h=0}$ . With this in mind, show that

$$\partial_t \zeta(t) = v \approx \kappa \frac{2\phi_+ h}{\gamma}. \quad (9)$$

Into which direction does the interface move?

e) Now, consider a curved interface and  $\mathbf{n}$  a normal vector on the interface. Then, the gradient on the interface can be written as

$$\nabla \phi = \mathbf{n} \partial_z \phi, \quad (10)$$

where  $\partial_z \phi$  is the derivative directed along the interface normal and  $z$  is the coordinate in normal direction (c.f. lecture). Then, one has

$$\nabla^2 \phi = \partial_z^2 \phi + \partial_z \phi \nabla \cdot \mathbf{n} \quad (11)$$

Restate the problem in exercise part d) for a gently curved interface of  $\phi_+$  enclosing  $\phi_-$  in 2D or 3D and show that

$$v = -\nabla \cdot \mathbf{n} + 2\kappa \frac{\phi_s h}{\gamma}. \quad (12)$$

When does this ansatz break down? In the lecture it was shown that all droplets will vanish. Does this still hold?

## Exercise 11 – Fisher-KPP equation

a) In this exercise, we consider a model that describes the spreading of a population  $u(x, t)$  through space. The model consists of an interplay between diffusion dynamics and local logistic growth:

$$\partial_t u(x, t) = D \nabla^2 u + \mu u(x, t) \left( 1 - \frac{u(x, t)}{K} \right) \quad (13)$$

with diffusion constant  $D > 0$ , linear growth/reproduction rate  $\mu > 0$ , and carrying capacity  $K$ . Show that by rescaling time, space, and the density  $u(x, t)$ , one obtains the following dimensionless form of the Fisher-KPP equation:

$$\partial_t u = \partial_{xx} u + u(1 - u). \quad (14)$$

b) It is, however, instructive to study the dimensionful equation 13, which we will consider throughout the exercise. Additionally, we specialize to a one-dimensional system. Identify the homogeneous stationary solutions of equation 13 and study their stability under a small plane-wave perturbation of the form  $e^{iqx + \sigma(q)t}$ . Derive the dispersion relations  $\sigma(q)$  in each case and classify stability.

c) For the rest of the exercise, we consider as initial condition of the Fisher-KPP equa-

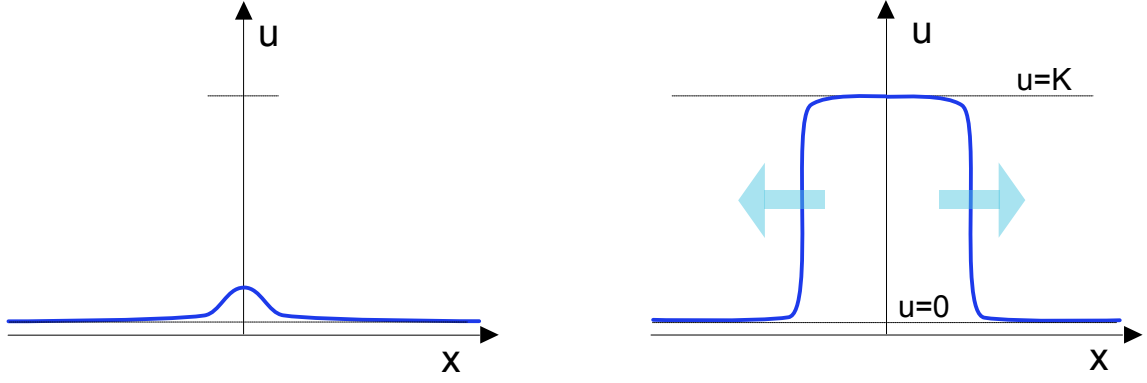


Figure 2: Left: the initial condition of the Fisher equation is a small perturbation localized in the center. Right: the initial perturbation grows and saturates at  $u = K$ , and the density  $u$  forms traveling fronts that move in the direction indicated by the blue arrow.

tion the configuration where  $u(x, t) = 0$  everywhere, apart from a small perturbation placed in the center (see figure 2). Argue why this perturbation will grow until  $u(x, t) = K$  and then spread through space in the form of a traveling front.

From dimensional analysis, argue that the traveling front connecting  $u = K$  to  $u = 0$  travels with speed  $c \sim \sqrt{D\mu}$  and has characteristic width  $\ell \sim \sqrt{D/\mu}$ .

**d)** In this exercise part, we will seek a traveling wave front of the form  $u(x, t) = a(\xi)$  with  $\xi = x - ct$  being the new coordinate of the moving frame, and  $c$  the constant speed of the traveling front. Here,  $a$  is the front solution that connects the two fixed points:

$$a(\xi \rightarrow \infty) = K, \quad a(\xi \rightarrow -\infty) = 0. \quad (15)$$

Show that  $a$  satisfies

$$Da'' + ca' + \mu a(1 - a/K) = 0,$$

and rewrite it as the first-order system

$$a' = b, \quad Db' = -cb - \mu a(1 - a/K). \quad (16)$$

Find the fixed points and the Jacobian of the equation above. Compute the eigenvalues at the fixed points. Finally, from the stability of the fixed points, argue why the velocity must satisfy  $c \geq 2\sqrt{D\mu}$ . *Hint: the trajectory in phase space—with  $a$  and  $b$  as axes—that connects the two fixed points exactly determines the shape of the interface.*

**e)** We now consider equation 17 in the region of space where  $u(x, t)$  is still approximately zero, i.e., far away from the traveling front. Linearize the equation around the fixed point  $u^* = 0$  and show that its time evolution follows:

$$u(\xi, t) = \int_{-\infty}^{+\infty} \frac{dq}{2\pi} e^{iq\xi + [iqc + \sigma(q)]t} \tilde{u}_0(q), \quad (17)$$

where  $\xi = x - ct$ ,  $\sigma(q) = \mu - Dq^2$ , and  $\tilde{u}_0(q)$  is the Fourier transform of the density at  $t = 0$ .

f) Take now the limit  $t \rightarrow \infty$  of expression 17 and discuss the condition on  $c$  such that the density does not diverge at large times. To perform the integral, use the saddle point approximation, which states that:

$$\int dx g(x) e^{-f(x)} \approx g(x_0) e^{-f(x_0)}, \quad (18)$$

where  $f(x), g(x)$  are arbitrary functions and  $x_0$  is a saddle point of  $f(x)$ , i.e.,  $\frac{d}{dx}f(x)|_{x_0} = 0$ . The two conditions that you should obtain from requiring that  $u(\xi, t \rightarrow \infty)$  does not diverge are:

$$c = i\sigma'(q_s) \quad \text{and} \quad c = \frac{Re[\sigma(q_s)]}{Im[q_s]},$$

where  $q_s$  is the saddle point, and  $Re$  and  $Im$  denote the real and imaginary parts of an expression. Show that solving these two equations yields  $c = 2\sqrt{D\mu}$ .

Your solutions should be handed in in moodle by **Wednesday, November 12<sup>th</sup> 2025, 10 am.**