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T VI: Nonlinear Dynamics and Complex Systems

(Prof. E. Frey)

Problem Set 7: Linear Stability analysis of pattern forming systems

Problem 1 *The Brusselator*

Consider an open system with the following reactions:

$$E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A, \quad C + A \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} B + D, \quad 2A + B \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} 3A, \quad A \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} F$$

We want to assume that the final products D and F are removed as soon as they are produced: $k_{-4} = k_{-2} = 0$. To simplify the analysis even further we assume $k_{-1} \cong 0$ (which is certainly justified as long as E is in excess) and $k_{-3} \cong 0$. Then we obtain the following rate equations:

$$\partial_t a = k_1 e - (k_2 c + k_4)a + k_3 a^2 b + D_a \nabla^2 a$$
$$\partial_t b = k_2 ca - k_3 a^2 b + D_b \nabla^2 b$$

a) Rescale the variables to obtain the dimensionless equations:

$$\begin{aligned} \partial_t a &= \varepsilon - (\mu + 1)a + a^2 b + d_a \nabla^2 a \\ \partial_t b &= \mu a - a^2 b + d_b \nabla^2 b \end{aligned} \tag{1}$$

b) Find the stationary states of the well-mixed system! Do the folllowing boundary conditions allow the stationary values as homogeneous distributions in space?

1. $a = a_0$, $b = b_0$ at the boundary (Dirichlet boundary conditions)
2. $(\hat{n} \cdot \overrightarrow{\nabla}) \begin{pmatrix} a \\ b \end{pmatrix} = 0$ (no-flux conditions; Neumann type)

c) Investigate the linear stability of the stationary state as homogeneous state in space:

$$a = a_0 + \Phi_a$$
$$b = b_0 + \Phi_b$$

The linearized version of (1) reads

$$\partial_t \overrightarrow{\Phi} = \mathcal{L} \overrightarrow{\Phi}, \tag{2}$$

with $\overrightarrow{\Phi} = 0$ or $(\hat{n} \cdot \overrightarrow{\nabla}) \overrightarrow{\Phi} = 0$ at the boundary, where $\mathcal{L}$ is a linear operator. Use the boundary conditions to find an ansatz for the n-th perturbation mode. Restrict to one spacial dimension. Calculate the eigenvalues λ_n.

d) Consider the modes with $Im(\lambda_n) \neq 0$ and sketch the crossover curve for μ as a function of the wavenumber. For which μ are all modes stable?

Problem 2 *Hydrodynamics of propelled hard rods: the impact of alignment interactions.*

Starting from a microscopic Langevin theory hydrodynamic equations for a fluid consisting of propelled hard rods can be derived (PRE 77, 011920, 2008). Propelled means that there is a force (mostly of microscopic origin), which drives each rod along its longitudinal axis. An opposing dissipating force gives rise to a constant velocity v_0 for each rod. The interaction between the rods is hardcore-repulsion only. The rods could align colinear (polar), as well as antiparallel. Both, the polar and antiparallel orientation is called a nematic configuration. On the level of the hydrodynamic equations the rods are descibed by a concentration field $c(\vec{x}, t)$ and a polarization field $\vec{P}(\vec{x}, t)$. A nematic configuration, commonly characterized by the nematic tensor, shall be ignored in this problem. A reduced version of equations Marchetti et.al. found is:

$$\partial_t c + v_0 \nabla \cdot (c\vec{P}) = D\nabla^2 c, \tag{3}$$

$$\partial_t (c\vec{P}) + \frac{1}{2} v_0 \nabla c = -D_R c\vec{P} + \eta \nabla^2 (c\vec{P}) + \xi \nabla\nabla \cdot (c\vec{P}), \tag{4}$$

where D_R, ξ, η and D are kinetic coefficients, all strictly positive defined.

a) Go through each term of the two equations above and explain its impact. Compare the equations above with the equations describing the flow of a ordinary fluid!

b) Investigate the fluctuations around the homogeneous concentrated, unpolarized state! For this linearize the equation around $c = c_0$ and $\vec{P} = 0$. Denote the pertubations as: $c = c_0 + \delta c$ and $\vec{P} = \delta\vec{P}$. Write the pertubations, e.g. δc, as Fourier-components with a growth rate s. Restrict to the longitudinal component $P_{||}$ defined longitudinal to the wavevector $\vec{k}$ as: $\delta\vec{P} = \vec{k}\delta P_{||}(\vec{k}, t) + \vec{k}_{\perp}\delta P_{\perp}(\vec{k}, t)$. Argue why!
Then derive the dispersion relation and determine the growth eigenvalues. What is the sign of the real part of each eigenvalues?
You will find two damping modes, which are called diffusive and propagating. Calculate the crossover from diffusive to propagating behaviour. Determine the velocity $v_{0,c}$ below which all modes are diffusive. Explain the impact of the rod velocity v_0.

c) Argue with the help of the underlying equations (without calulations) the stability of the homogeneous concentrated, polarized state, e.g. $\vec{P} = \vec{P}_0 + \delta\vec{P}$.

d) Now imagine that the constant D_R to be a function of the concentration: $D_R = D_{R,0}(c_c - c)/c$. A term proportional to $+\vec{P}$ corresponds to a microscopic mechanism trying to align the rods in a polar configuration – the alignment interaction. Discuss the stability of the homogeneous concentrated, unpolarized state (no calculations)! Would you conclude that the polarized state is now stable? Why not?

e) Extend the equation for the polarization with $-\beta P^2 \vec{P}$ on the right hand side and the concentration dependent D_R of part d.). Determine the base state for the polarization field P_0. Assume $\vec{P}_0 = P_0\vec{k}$ and consider $P_{||}$ as in b.). Show by calculation that the homogeneous concentrated, P_0 – polarized state is now stable for $c > c_c$ and for all wavenumbers! For simplicity ignore fluctuations in density ($\delta c = 0$). Discuss the meaning of the crossover $s = 0$.

Hint: When treating the system numerically one finds an inhomogeneous moving stripe pattern of polar rods (see preprint arXiv:1001.3334). But note that a further term, the convective term $\vec{P}\cdot\nabla(c\vec{P})$, which is non-linear, appears to be essential for the emergence of those polarized stripe patterns. This is beyond the scope of the linear stability analysis.