Institute for Theoretical Physics — Heidelberg University
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Nonlinear dynamics — Summer term 2024

(Last) Assignment 11

Handout 01.07.2024 – Return 08.07.2024 – Discussion 11./12.07.2024

Exercise 1 [6 points]: Reaction-diffusion systems: Turing instability

Consider the brusselator model

$$\begin{aligned}\partial_t u &= D_u\partial_x^2 u + a - (b+1)u + u^2 v,\\ \partial_t v &= D_v\partial_x^2 v + bu - u^2 v,\end{aligned}$$

where $u(x,t)$, $v(x,t)$ are concentration fields.

1. Determine the homogeneous stationary base state (with $u \neq 0, v \neq 0$). *(1 point)*
2. Calculate the onset of the finite wavelength (Turing) instability, as discussed for the general case in the lecture. *(4 points)*
   HINT: In the eigenvalue problem, it is again enough to study $\sigma = 0$. Solve for the control parameter $b(q)$, minimize with respect to q and show that you get $b_c^{\text{Turing}} = (1 + a\sqrt{D_u/D_v})^2$ and $q_c = \sqrt{\frac{a}{\sqrt{D_u D_v}}}$.
3. To observe the finite wavelength pattern, the control parameter b needs to be beyond b_c^{Turing} but below the threshold of the other instability occuring in the system, the oscillatory Hopf instability having $b_c^{\text{Hopf}} = 1 + a^2$ (see lecture). What restriction do b_c^{Turing} and b_c^{Hopf} hence imply for the diffusion coefficients of the two species? *(1 point)*

Exercise 2 [9 points]: Soliton warm-up: the Fermi-Pasta-Ulam problem and the KdV equation

In an attempt to study thermal equilibration in a “real” solid, in the 50’s Fermi and coworkers studied a 1D chain of nonlinear springs,

$$m\frac{d^2 y_n}{dt^2} = k\left[(y_{n+1} - 2y_n + y_{n-1}) + \alpha(y_{n+1} - y_n)^2 - \alpha(y_n - y_{n-1})^2\right]. \tag{1}$$

They found no equilibration, but rather that only a few modes get exited. Later in 1962-65, Zabusky and Kruskal applied a continuum approximation to Eq. (1) for small nonlinearity α and derived the Korteveg-de Vries equation (KdV) from it,

$$\partial_t u + u\partial_x u + \gamma\partial_x^3 u = 0, \tag{2}$$

which is one of the most important equations displaying *solitons* as solutions.

1. Motivate/derive Eq. (1) by considering the forces acting from right and left on a bead between two nonlinear (cubic potential) springs. *(1 point)*

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2. Make a continuum approximation by assuming $x_n = nh$ and $y_n = y(x_n)$, with h the lattice spacing. Then perform a Taylor series (assuming h and α are small) to get

$$m\partial_t^2 y = k\left[h^2\partial_x^2 y + \frac{h^4}{12}\partial_x^4 y + 2\alpha h^3\left(\partial_x y\right)\left(\partial_x^2 y\right) + \mathcal{O}(\alpha h^5)\right]. \tag{3}$$

   In leading order, this is a linear wave equation. What is the linear wave speed v? *(3 points)*

3. Now transform into the frame of a right-traveling wave, including a slow time scale T, by writing:

$$X = x - vt\,,\;\; T = \alpha h v t. \tag{4}$$

   Show that this transforms the derivatives into *(1 point)*

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial X}\,,\;\; \frac{\partial}{\partial t} = -v\frac{\partial}{\partial X} + \alpha h v\frac{\partial}{\partial T}. \tag{5}$$

4. Use the transformation to derive the KdV equation for the variable $u = \frac{\partial y}{\partial X}$. *(3 points)*

5. The KdV equation has soliton solutions. Use this knowledge to explain the result Fermi obtained numerically for small systems: i.e. that beginning with one (linear) mode excited initially, one does not get equilibration but rather a few excited modes that are localized and travel through the system. *(1 point)*

THE NEXT PROBLEM IS FOR THOSE INTERESTED IN NUMERICS. IT CAN EITHER BE USED TO REPLACE ONE OF THE OTHER PROBLEMS ON THIS SHEET OR CAN BE USED TO GET BONUS POINTS. YOU CAN TURN IT IN LATER IF NEEDED, UNTIL THE LAST TUTORIAL.

Replacement/Bonus Exercise [8 points]: Pseudo-spectral method for Swift-Hohenberg model

Here we want to numerically study the Swift-Hohenberg model for $u(t,x)$,

$$\partial_t u = \left[\epsilon - (q_0^2 + \partial_x^2)^2\right] u - u^3\,, \tag{6}$$

with periodic boundary conditions. As we are looking for periodic patterns, it is advantageous to solve in Fourier space. However, the equation is nonlinear, which implies computationally costly convolutions. Hence we use the so-called *operator-split pseudo-spectral method*, as explained now:
The idea is to separate the right hand side of the equation into two parts, a linear operator[1], $\mathcal{L}u = \left[\epsilon - (q_0^2 + \partial_x^2)^2\right] u$, and a nonlinear operator, $\mathcal{N}(u) = -u^3$. We then treat both parts seperately and one after the other, the nonlinearity in real space (to avoid convolutions) and the linear operator in Fourier space (to take advantage of periodicity).
First, we integrate the nonlinear term (here with simple Euler stepping), as if this were the only term:

$$\partial_t u = \mathcal{N}(u) = -u^3, \quad \text{for initial data:} \quad u(t,x). \tag{7}$$

Integrating this equation one timestep Δt will produce some intermediate field that we will denote as $\tilde{u}_t$. This field we use as initial data for the second evolution problem, in which only the linear operator appears

$$\partial_t u = \mathcal{L}u = \left[\epsilon - (q_0^2 + \partial_x^2)^2\right]\, u, \quad \text{for initial data:} \quad \tilde{u}_t. \tag{8}$$

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[1] The linear operator must contain the highest-order spatial derivatives for the method to work properly.

We (spatially) Fourier transform $\tilde{u}_t$, solve equation (8) in Fourier space (hence the name spectral method) and transform back.
The result we get from both steps together is then $u(t + \Delta t)$.
In short the algorithm reads:

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Initialize $u(t, x)$ with random data (of small amplitude, around $u = 0$).
Define the wave numbers $q$ for the Fourier modes to consider.
Then iterate:
    1) Calculate $u - dt\, u^3$ (in real space).
    2) Discrete Fourier transform the result of 1).
    3) Apply time evolution with linear operator on result of 2).
    4) Backtransform result of 3) into real space.
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We delivered a Python Jupyter notebook, see *SH_exercise.ipynb* with more detailed instructions. Solve the following tasks in this notebook and hand in your solution as a PDF of your notebook after running all cells. (Alternatively, you can also use mathematica, maple etc. using their Fourier transforms. Then please read the pdf summary of the jupyter notebook, also available on the uebungsgruppen, for the detailed instructions.)

1. Implement the random initialization of $u(t = 0, x)$.
   Answer the question why it does not matter whether we use the wave numbers $q_n = 2\pi n/L$ for $n \in \left\{-\frac{N}{2}, \ldots, -1, 0, 1, ..., \frac{N}{2} - 1\right\}$ or for $n \in \{0, 1, \ldots, N\}$.
   Then show that in Fourier space, for the linear part of the SH equation the time evolution from initial condition $\hat{u}(t, q_n)$ for a timestep Δt and wavenumber q_n is given by

   $$\hat{u}(t + \Delta t, q_n) = \exp\left(\left[\epsilon - (q_0^2 - q_n^2)^2\right] \cdot \Delta t\right) \cdot \hat{u}(t, q_n) \tag{9}$$

   and implement it. *(3 points)*

2. Implement the full operator-split pseudo-spectral method in one dimension, cf. the algorithm box above. *(2 points)*

3. Plot the one dimensional simulation data for $q_0^2 = 1$ and $\epsilon = 0.1$ as a 3D surface plot of $u(x, t)$ and for a few interesting times t as $u(x)$. *(2 points)*

4. Plot the squared amplitude A^2 of your obtained pattern as a function of simulation time for $\varepsilon = 0.1$ to check whether your simulation has converged. Then determine the final squared amplitudes of simulated patterns for $\epsilon = 0.05,\ 0.1,\ 0.2,\ 0.3,\ 0.4,\ 0.5$ and plot your numerical results for A^2 as a function of ϵ alongside the theoretical expectation from the amplitude equation. *(1 point)*