Homework 7: Molecular systems

1. Consider the chemical reaction: $A + 2B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C + D$

   (a) Write down the rate of this chemical transformation expressed in the rates of individual components A, B, C, and D.

   (b) Write down the actual rate of the reaction.

   (c) Write down the rates of change of each of the chemicals.

   (d) What does the equilibrium constant equal to?

   (e) Write down the stoichiometric matrix.

2. Consider a bi-stable system:

$$\begin{aligned} x' &= y \\ y' &= -ay + b(x - x^3) \end{aligned}$$

   Recall that bi-stable systems have two stable steady states, which are usually separated by a saddle. This systems is not an exception. The goal of this exercise to show the switching effect of different initial conditions.

   (a) Find three steady states.

   (b) Prove one of them is a saddle, whereas two others are stable spirals or nodes (determine parameter conditions for being spirals and nodes), given positive parameters a and b.

   (c) Choose parameters a and b so that there are two co-existing spirals and $0 < a \leq 1$, $0 < b \leq 1$ and simulate for a series of initial conditions. For that, generate matrix of `n` initial conditions `x0` (`2 x n`), say, located on the positive part of the X-axis (e.g. at Matlab prompt: `x0=[linspace(0,5,n); zeros(1,n)]`, where `n=100` or so. (You can generate initial conditions randomly or according to some rule in any sub-region around the steady states.) Then simulate the system for each initial condition `x0(:,ii)` (where `ii` runs from 1 to `n`) and plot the phase portrait (all trajectories on the same plot), using `ode45` and `plot` commands. (*Hint:* use `for` loops or vectorizing techniques, make final simulation time equal 50, that's enough.)

(d) Try to trace which attractor the trajectories land on. If the subregions of the phase space were big enough, you must see closely located initial conditions leading to different attractors.

(e) You can further color trajectories landing on one attractor with one color (e.g. red), whereas other trajectories landing on the other attractor with another color (e.g. blue). You must see red-blue bands circulating around the steady states like on the figure below: