

CHEMISTRY 410/510

NONLINEAR DYNAMICS & CHAOS: WINTER, 2007.

Name: _____ Social Security No. _____

MID-TERM EXAMINATION *February 28, 2007 [8 a.m. - 10:00 p.m.]*

This exam has three questions, with choice of either A or B (not both) for the second and third questions. There is a bonus question which students do not have to attempt for full credit.

Question 1 [40 points]

As succinctly as you can, define the following terms that are used in the collective study of nonlinear dynamics. Where possible, qualify your definition with an appropriate equation.

(a) Mathematical definition of chaos

(b) Feigenbaum number

(c) Marginal stability

(d) Poincare-Bendixson theorem

(e) a deterministic system

(f) separatix

(g) bifurcation

(h) accumulation point

(i) distinguishing between chaos and noise

(j) attractor

Question 2 [30 points]

Attempt EITHER A or B (not both)

Part A

- (a) A damped oscillator has the following equation:

Is this a linear or nonlinear system? The swinging pendulum is given by the equation $d^2x/dt^2 + (g/L)\sin x = 0$. Evaluate also, if this is linear or nonlinear.

- (a) From the initial value problem $dx/dt = x + y$; $dy/dt = 4x - 2y$; Find the eigenvalues and eigenvectors for this system. Draw a rough phase portrait for dynamical system that has the eigenvalues you calculated for this problem.
- (b) For a flow system with chemical kinetics governed by cubic autocatalysis; $A + 2B \xrightarrow{k_3} 3B$ (rate constant k_3), prove that this system will always have three steady states and also evaluate the relevant Jacobian.

Part B

One of the most well-studied nonlinear systems is the nonlinear electrical circuit which involves a series connection of an inductor, a diode and a signal generator. Describe fully the mechanism of such a system: the effect of the diode and the inductor, the type of data obtained, and the control parameters (normally) utilized to study the system. Next report on the bifurcation sequence observed. Does the system show chaos? [this is the 'whole nine yards']

Question 3 [30 points]

Attempt EITHER A or B (not both)

Part A

- (a) Consider the logistic map: $X_{n+1} = rX_n(1-X_n)$. Decomposition of the map at any value of the bifurcation parameter that leaves the value of X invariant is called a fixed point. Prove that this map will always have two fixed points and evaluate them. (r is a bifurcation parameter which is sometimes represented by 'A').
- (b) Following up from (a), above, one can have a little fun with this map and predict, precisely the fixed points on the basis of the bifurcation parameter. Otherwise, one has to go through cumbersome iterations to find these points. Find the sets of fixed points generated by $r = 0.5, 1.0, 2.5$ and 3.0 . Roughly sketch the unimodal map and show how these fixed points will be attained from a seed value of $X_0 = 0.5$ ($f(X_n)$ normalized in the interval). Next, use these symbolic dynamics to roughly sketch the appearance of the time series traces that might accompany such decompositions.

- (c) Now for some heavy lifting. Assume a seed value of 0.500, and a bifurcation parameter, $\delta = 3.10$. Perform no more than 6 iterations. What pattern (if any) emerges? Another 6 iterations at $\delta = 3.45$; what do you see? Are we in chaos yet?

Part B

- (a) The most thoroughly-studied chemical oscillator is the Belousov-Zhabotinski reaction. What is the ‘driving’ reaction for the BZ system? [you need to describe the overall reaction occurring as well as its stoichiometry].
- (b) The most widely-accepted mechanism for the BZ reaction is the FKN mechanism which is made up of three parts: A, B, and C. Name these parts and their roles (i.e. the major activity in each part). Write down the chemical reactions that make up these parts.
- (c) Give a detailed description of Processes A and B and how they interact by invoking bromide ion control. What are the critical concentrations of bromide and how do they affect the overall dynamics of the BZ reaction system.

Bonus Question [Need not be attempted for full credit; 10 points]

Romeo is in love with Juliet, but not in mode of the classic Shakespeare tale. In the Chem 510 version, Juliet is very fickle: the more Romeo loves her, the more Juliet wants to run away and hide. But when Romeo gets discouraged and backs off, Juliet begins to find him attractive (happens all the time doesn’t it?). Romeo, in turn, echoes Juliet: he warms up when she loves him and grows cold when she hates him. This is going to quite a wild ride!!!!!!!

Let $\mathbf{R}(t)$ be Romeo’s love/hate for Juliet at time t , and $\mathbf{J}(t)$ that of Juliet for Romeo.

The model then generated for the star-crossed romance is:

$$d\mathbf{R}/dt = a\mathbf{J}$$

$$d\mathbf{J}/dt = -b\mathbf{R}$$

(both a , and b are positive, by definition).

Predict the dynamics generated by this romance. Can a steady state be ever achieved? May be a limit cycle? If this is a limit cycle, is it stable? Will ever a time arise when both Romeo and Juliet are madly in love with each other (simultaneously)? And, if a time arises when they both hate each other, what force will draw them to the attracting limit set? Will they ever get married?

[Strogatz, *S. H. Math. Magazine* 1988, 61, 35]