12 Nonlinear Dynamics/Dynamical Systems

12.8 A Nonlinear Map and the Dynamics of Hydrogen Atoms in Electric Fields (7 units)

Material in both the Part II course Dynamical Systems and the Part II course Classical Dynamics is relevant to this project.

1 Part 1

The behaviour of Rydberg atoms, i.e. atoms in highly excited electronic states, in the presence of external fields has been the subject of extensive investigations. Advances in theoretical and experimental techniques in the past few decades have made it possible to study the dynamics of hydrogen atoms with very high initial quantum number. In this limit, and because of the form of the potential, they are ideal candidates for exploring the borderline between classical and quantum mechanics.

This projects explores a simple dynamical model, used to approximate the particular case of hydrogen atoms in a monochromatic, linearly polarised electric field, which are initially prepared in a very extended state along the field direction.

This case can be modelled using classical dynamics, by the one-dimensional Hamiltonian

$$H(x,p,t) = \frac{p^2}{2} - \frac{1}{x} + \varepsilon x \sin \omega t \tag{1}$$

where p and x are momentum and position of the electron, and ε and ω are strength and frequency of the external electric field. It is convenient to express this Hamiltonian in action-angle variables (I, θ):

$$H(I,\theta,t) = -\frac{1}{I^2} + \varepsilon \left[\frac{3I^2}{2} - 2I^2 \sum_{s=1}^{\infty} \frac{J_s'(s)}{s} \cos(s\theta) \right] \sin \omega t \ , \tag{2}$$

where $J_s'(z)$ denotes the derivative of an ordinary Bessel function and the term in square brackets is the Fourier expansion of $x(I,\theta)$.

The equations of motion are then

$$\begin{aligned} \dot{I} = -\frac{\partial H}{\partial \theta} &= \varepsilon \sin \omega t \, \frac{\partial x(I,\theta)}{\partial \theta} \\ \dot{\theta} = \frac{\partial H}{\partial I} &= \frac{1}{I^3} - \varepsilon \sin \omega t \, \frac{\partial x(I,\theta)}{\partial I} \quad . \end{aligned} \tag{3}$$

By integrating these equations over one field period, we can obtain the solution in the form of a discrete map.

In the unperturbed case $\varepsilon = 0$ we obtain the simple twist map

$$\begin{aligned} I_{n+1} &= I_n \\ \theta_{n+1} &= \theta_n + \frac{2\pi}{I_{n+1}^3} \quad , \end{aligned} \tag{4}$$

while for $\varepsilon \neq 0$ the solution has the form

$$\begin{aligned} I_{n+1} &= I_n + f(I_{n+1}, \theta_n, \varepsilon) \\ \theta_{n+1} &= \theta_n + \frac{2\pi}{I_{n+1}^3} + g(I_{n+1}, \theta_n, \varepsilon) \quad . \end{aligned} \tag{5}$$

The functions f and g have no known analytical form. We could find an approximate solution by truncating the sum in (2), but for the purpose of this simple model we shall only require that: (a) the fixed points of the perturbed map are the same as, or very close to the fixed points of the unperturbed twist map; (b) the perturbed map is area-preserving; (c) the motion described by the perturbed map becomes 'chaotic' only above a critical value of the action I, which depends on the strength of the perturbation. Chaotic motion is that for which trajectories, i.e. iterated points of the map, do not lie on any invariant curve.

We shall therefore choose $f = -\frac{\partial \mathcal{B}}{\partial \theta_n}$ and $g = \frac{\partial \mathcal{B}}{\partial I_n}$, with $\mathcal{B} = \varepsilon^{I_{n+1}^{-2}} \cos\theta_n$. and study the map

$$\begin{aligned} I_{n+1} &= I_n + \varepsilon^{I_{n+1}^{-2}} \sin\theta_n \\ \theta_{n+1} &= \theta_n + \frac{2\pi}{I_{n+1}^3} - 2\frac{\log\varepsilon}{I_{n+1}^3}\varepsilon^{I_{n+1}^{-2}} \cos\theta_n \quad . \end{aligned} \tag{6}$$

> **Question 1** Check that the fixed points of the perturbed map (6) are very close to those of the simple twist map (4).
>
> By considering how the perturbed map (6) can be described as a transformation with a generating function of the form $F_2(I_{n+1}, \theta_n)$, check that it is area-preserving (why do we need this?).

Now write a program that plots trajectories of the perturbed map (6) in phase space. Calculate θ_n modulus 2π. Note that I_{n+1} is defined implicitely in terms of I_n, so you will need to use some root-finding method to calculate it at each step.

> **Question 2** For two different value of the field parameter: $\varepsilon = 0.0005$ and $\varepsilon = 0.002$, plot several phase space trajectories of the map (.) on the same graph. In each case look for representative trajectories with I in the range $[0.7, 2.0]$, for example starting at $I = 0.81$. Can you restrict initial values of θ to the range $[0, \pi]$?
>
> Comment on your choice of root-finding method, and the numerical error it introduces. Comment on your choice of initial conditions, and total number of iterations.
>
> Estimate the complexity of your program.
>
> Describe the structure of the phase space. Give an estimate, based on the observed behaviour, of the critical value of I above which chaotic regions of phase space exist.

Now iterate the map with several values of the field parameter in the range $\varepsilon \in [0, 0.1]$

> **Question 3** Plot phase space trajectories for some representative values of ε.
>
> Describe how the phase space structure changes as a function of ϵ. Find how the critical value of I changes with ϵ. Comment on the number of iterations needed to show a good illustration of the behaviour.

2 Part 2

In this section we introduce a function that models a slow change of the field parameter ε, in order to explore the existence of adiabatic invariants in the non-integrable system under investigation. A similar problem is investigated in [3].

Adapt the program of Part 1 to iterate the perturbed map, but this time with a gradual 'switch-on' of the perturbation, using the discrete switch-on function defined by:

$$A(n, N_a) = \begin{cases} 0 & s \leqslant 0 \\ s^2(2-s^2)^2 & 0 < s < 1 \\ 1 & 1 \leqslant s \end{cases}, \tag{7}$$

where N_a is the length (in number of steps) of the adiabatic switch, and $s = n/N_a$.

> **Question 4** In the cases $\varepsilon = 0.005$ and $\varepsilon = 0.015$ repeat plots of the iterates of the maps for a range of initial conditions as in question 3, but now using the function $A(n, N_a)$ to switch on the perturbation, with $N_a = 100$. Describe the effects of switching on the perturbation gradually.

Focus now on just two initial values of the action: $I = 1.1$ and $I = 1.236068$,

> **Question 5** Plot results obtained with different lengths of the adiabatic switch, for example $N_a = 10, 100, 500, 1,000, 2,000$ (or other values that you think best illustrate the dependance), and varying the number of total iterations of the map.
>
> Describe how persistence of the invariant curves varies with the different parameters.

We can verify adiabatic invariance by using the non-adiabaticity parameter defined by Dana and Reinhardt (1987):

$$\Delta J(N_a) = \left[\frac{1}{2\pi}\int_0^{2\pi} (I_{N_a}(\theta) - I(\theta))^2 d\theta\right]^{1/2}. \tag{8}$$

Write a programme to calculate numerically the non-adiabaticity parameter $\Delta J(N_a)$ using a suitable numerical approximation for the integral.

> **Question 6** Comment on your choice of approximation for the integration.
>
> Show plots of $\Delta J(N_a)$ v N_a for all the cases in Question 5.
>
> Use the non-adiabaticity parameter to verify cases where adiabaticity holds, and where it breaks down.
>
> Comment on the relevance of these results to quantisation of this classical system.

References

[1] Casati, G., Guarnieri I. and Shepelyansky D. L. 1988 *IEEE Journal of Quantum Electronics*, 24, 1420.

[2] Lichtenberg, A. J. and Lieberman M. A. *Regular and Stochastic Motion* Springer

[3] Dana, I and Reinhardt W. P. 1987 *Physica D*, 28, 115.