Periodic theory approach to classical dynamics in a two-dimensional chaotic double well

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We study some aspects of the classical dynamics of a particle in a double well, which shows chaotic behavior for certain energies. The dynamics in a double well is still an open problem in two or higher dimensions. Here we use periodic orbit theory to calculate the diffusion coefficient using the cycle expansion methods. We work in the full domain with a 4-symbols simbolic dynamics to find periodic orbits for energies just above the saddle point of the potential energy.

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I. INTRODUCTION

One dimensional quantum double well tunneling has been studied throughly, although for higher dimensions this is still an open problem. We intend to study this problem with periodic orbit theory, and we begin here by studying the classical counterpart to gain some understanding of the dynamics of the system.

The periodic orbit theory of classical chaos is a very robust tool for studying chaotic dynamical systems. The theory expresses all long time averages over chaotic dynamics in terms of cycle expansions [1?], sums over periodic orbits ordered hierarchically according to the orbit length, stability, or action. If the symbolic dynamics is known, and the flow is hyperbolic, longer cycles are shadowed by the shorter ones, and cycle expansions converge exponentially or even super-exponentially with the cycle length [3].

II. PROBLEM AT STUDY

We choose a potential for which its quantum dynamics has been studied in Ref. [2]. This potential showed chaotic behavior for the parameter $/miu = 0.1$, which is the value that we employ. This potential

$$V(x, y) = (x^2 - 1)^4 + x^2y^2 + \mu y^2 \quad (1)$$

is shown in Figs. 1 and 2.

It has two global minima in x for $x = \pm 1$ and $y = 0$, global minima in y for $y = 0$ and a saddle point for $(x = 0, y = 0)$.

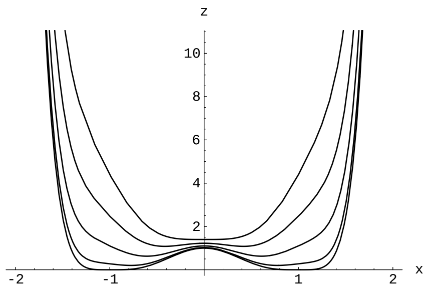

FIG. 1: The potential for $y = 0, 0.5, 1.0, 1.5, 2.0$

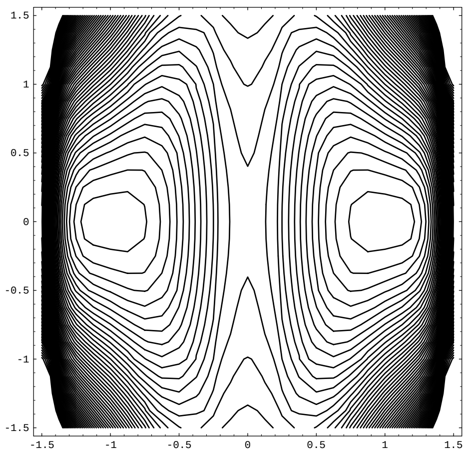

FIG. 2: Contour plot of the potential in the plane x-y. This potential has two minima at $(x, y) = (\mp 1, 0)$ and a saddle point in $(x = 0, y = 0)$

In sect. II, the set of ordinary differential equations which govern the evolution of a particle in the well are derived. The symbolic dynamics used to describe the trajectories and the Poincare sections choosen are discussed. In sect. **??**, the multishooting rutine implemented to search for periodic cycles is explained. Also, the periodic orbit expansion is implemented to calculate the diffusion coefficient for this system. My results are summa-

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rized,discussed and possible improvements of the method in sect. III. The setbacks for explained in appendix A.

A periodic orbit is a solution (x, T), $x \in \mathbb{R}^d$, $T \in \mathbb{R}$ of the *periodic orbit condition*

$$f^T(x) = x\,, \qquad T > 0 \tag{2}$$

for a given flow or discrete time mapping $x \mapsto f^t(x)$. Our goal is to determine periodic orbits of flows defined by first order ODEs

$$\frac{dx}{dt} = v(x)\,, \qquad x \in \mathcal{M} \subset \mathbb{R}^d\,, \qquad (x, v) \in \mathbf{T}\mathcal{M} \tag{3}$$

in d dimensions. Here $\mathcal{M}$ is the phase space (or state space) in which evolution takes place, and the vector field $v(x)$ is smooth (sufficiently differentiable) almost everywhere.

A. Equations of Motion

Here we derive Hamilton's equations of motion and the equations of variations for the system.

The Hamiltonian for our system is

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + (x^2-1)^4 + x^2y^2 + \mu y^2 = E. \tag{4}$$

Using

$$\begin{aligned} \dot{q} &= +\frac{\partial H}{\partial p} \\ \dot{p} &= -\frac{\partial H}{\partial q} \end{aligned} \tag{5}$$

we can find the equations of motion governing our system:

$$\begin{aligned} \dot{x} &= \frac{p_x}{m} \\ \dot{y} &= \frac{p_y}{m} \\ \dot{p_x} &= -8x(x^2-1)^3 - 2xy^2 \\ \dot{p_y} &= -2yx^2 - 2x\mu y \end{aligned} \tag{6}$$

For a given energy E, the initial conditions have to be in a certain range. The maximum $|x_{max}|$ is obtained for zero kinetic energy and zero displacement in y:

$$\begin{aligned} (x^2-1)^4 &= E \\ x_{max} &= \pm\sqrt{E^{\frac{1}{4}}+1} \end{aligned} \tag{7}$$

The maximum value $|y|$ can have for any $x < |x_{max}|$, having total energy E, is obtained by setting the kinetic energy to zero.

$$\begin{aligned} (x^2+1)^4 + x^2y^2 + \mu y^2 &= E \\ y^2(x^2+\mu) &= E - (x^2+1)^4 \\ y &= \pm\sqrt{\frac{E-(x^2-1)^4}{x^2+\mu}} \end{aligned} \tag{8}$$

The initial positions for a given energy E satisfy:

$$\begin{aligned} |x| &\leq \pm\sqrt{E^{\frac{1}{4}}+1} \\ |y| &\leq \pm\sqrt{\frac{E-(x^2-1)^4}{x^2+\mu}} \end{aligned} \tag{9}$$

$$\tag{10}$$

with the magnitude of maximum momemtum $\overrightarrow{p}$ given by

$$\begin{aligned} \frac{p^2}{2m} &= E - (x^2-1)^4 - x^2y^2 - \mu y^2 \\ |p| &= \sqrt{2m(E-(x^2-1)^4 - x^2y^2 - \mu y^2)} \end{aligned} \tag{11}$$

If we define θ as an angle with respect to the horizontal, the initial p_x and p_y for these initial positions and energy are

$$\begin{aligned} p_x &= \sqrt{2m(E-(x^2-1)^4 - x^2y^2 - \mu y^2)}\cos(\theta) \\ p_y &= \sqrt{2m(E-(x^2+1)^4 - x^2y^2 - \mu y^2)}\sin(\theta) \end{aligned} \tag{12}$$

We intend to find periodic orbits within specific energy shells.

B. Symbolic Dynamics

Cycle expansion requires periodic orbits to be order according to length. This is why we need a mechanism that helps order and differentiate cycles. Symbolic dynamics and Poincare sections together are a very useful tool for this matter for characterizing trajectories. A Poincare section is a $d-1$-dimensional in phase space, which is described by a unique symbol. Every time a trajectory hits a Poincare section its corresponding symbol is appended to it symbol sequence. The Poincare sections should be choosen in a way as to produce a 1-1 correspondence between words in the symbolic dynamics and periodic cycles. No cycle should have two sequences describing it, nor should a word describe two cycles. With this in mind, we looked for the appropiate Poincare sections to describe our dynamics.

Since our potential is symmetric in the x-axe, we started with two Poincare sections: R and L relating p_x and x. Poincare section R was croosed whenever p_x passed from positive to negative for $x > 0$, while Poincare section L was crossed when p_x went from positive to negative for $x < 0$. After integrating the ODE system and looking at the dynamics of the particle in the double well, we realized that our symbolic dynamics did not differentiate between cycles not symmetric in the y-axe.

For instance, in Fig. **??** we can see a trajectory not symmetric in the y-axe. Although we don't currently know if this cycle exist, in case it does, our symbolic dynamics did not describe it well. For this trajectory, when the particle returns to the origin it has an opposite p_y as

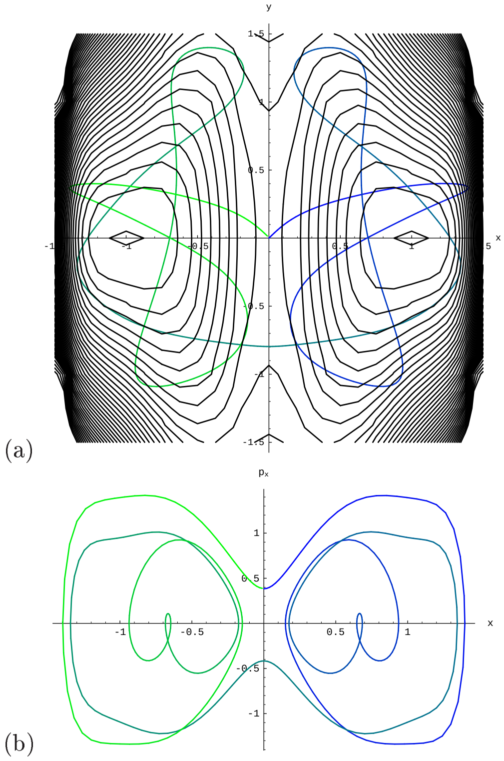

FIG. 3: (a)Trajectory not symmetric in the y-axe.(b) Phase space plot: p_x vs x

it initially had, so it would continue with a mirror trajectory with respect to the x-axe. According to our symbolc dynamics this would resemble a cycle $\overline{RRRRLLLL}$, which has period 8, but it really is a cycle of period 16, $\overline{RRRRLLLLRRRRLLLL}$.

After this initial approach, we decided to switch to the fundamental domain ($x \geq 0$ and $y \geq 0$) with a different symbolic dynamics, X and Y, which described bounces on the x-axes and on the y-axes, respectively. It appeared to describe well our system but the origin could not be handled easily. We thought of giving the origin an extra symbol to characterize trajectories crossing the origin. Depending on the precision, a trajectory appearing to cross the origin, could touch either axe. So we decided to return to the full domain and leave the fundamental domain for later when we know more about the dynamics of the system.

Finally, we decided to use 4 symbols to describe the trajectories on our double well.
R: when p_x crosses from positive to negative.
L: when p_x crosses from negative to positive.
U: when p_x crosses from positive to negative.
D: when p_x crosses from negative to positive.

The symbol R (L) denotes bounces on the right(*left*) wall of either well, while symbol U (D) describes bounces on the upper(*down*) wall of either well.

The shortest cycles are of length 2: $\overline{RL}$ for horizontal bounces along $y = 0$ and $\overline{UD}$ for bounces along $x = 0$.

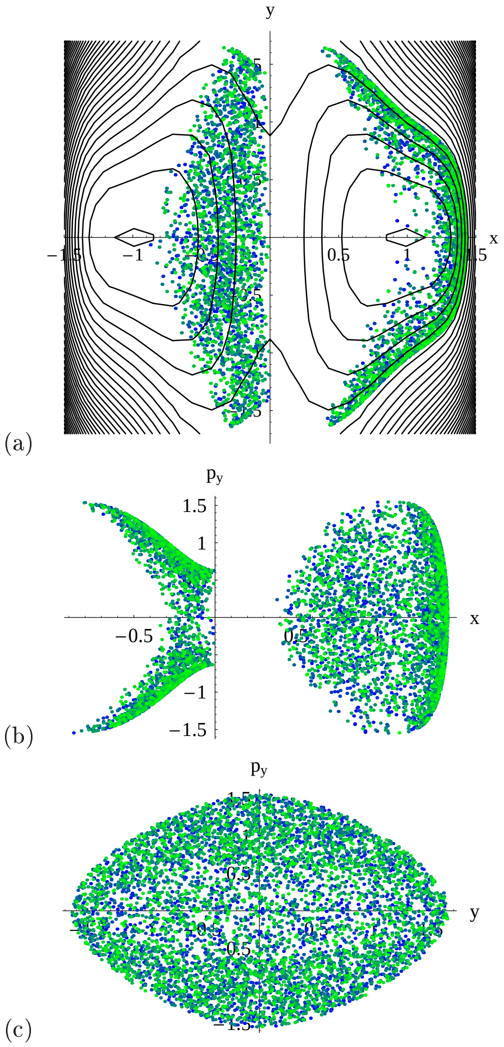

FIG. 4: Configuration and phase space plots for Poincare section R (p_x changes from positive to negative) for a particle with energy $E = 1.2$ and initial phase space position ($x = 1.0$, $y = 0.1$, $p_x = 0.0$, $p_y = 1.0$) (a) x vs y (b) x vs p_y (c) y vs p_y

From then on, we only have some guesses as to where cycles. We haven't been able to locate non trivial periodic cycles, becuase of the chaotic behvior of the trajectories. The next smallests cycle could be an ellipse bouncing between the two wells, $\overline{RULD}$ of period 4, and an ∞-shape between the two wells, $\overline{RUDLUD}$ of period 6. But we still have to see if these cycles really exist.

The Poincare sections R and U for a particle with initial conditions ($x = 1.0$, $y = 0.1$, $p_x = 0.0$, $p_y = 1.0$) are presented in Figs. **??** and **??**. Poincare section L, is the reflection of Poincare section R with respect to the y-axe. A similar reflection relates Poincare sections U and D.

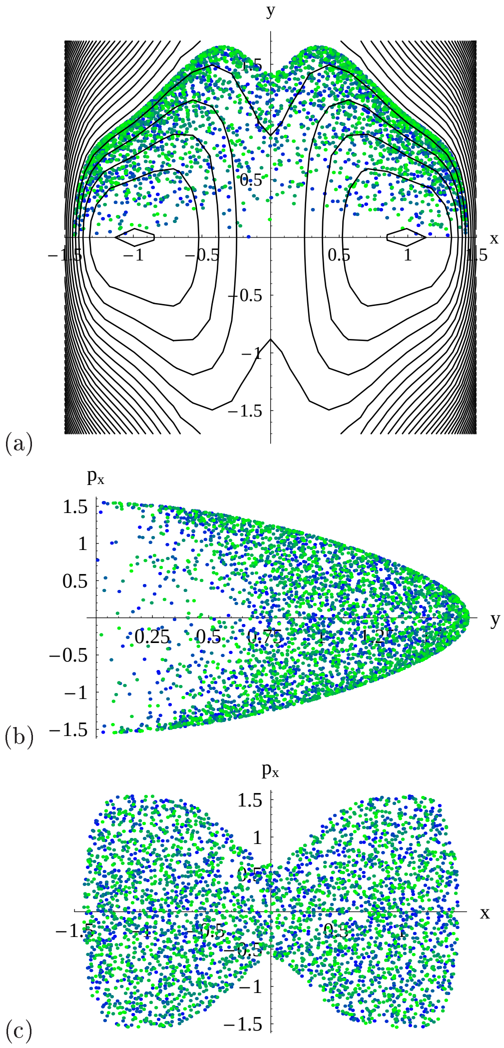

FIG. 5: Configuration and phase space plots for Poincare section U (p_y changes from positive to negative) for a particle with energy $E = 1.2$ and initial phase space position ($x = 1.0$, $y = 0.1$, $p_x = 0.0$, $p_y = 1.0$) (a) x vs y (b) y vs p_x (c) x vs p_x

C. Finding Periodic Orbits

The method for finding cycles and applying periodic orbit theory to Hamiltonian flows is outlined by Cvitanovich in **??**. Let $x(t) = f^t(x)$ be the state of the system at time t obtained by integrating (6), and $J(x,t) = dx(t)/dx(0)$ be the corresponding time-dependet Jacobian obtained by integrating

$$\frac{dJ}{dt} = AJ\,, \quad A_{ij} = \frac{\partial v_i}{\partial x_j}\,, \qquad \text{with } J(x,0) = \mathbb{1}\,. \quad (13)$$

In our case, A is given by

$$\mathbb{A} \;=\; \begin{pmatrix} 0 & 0 & \frac{\partial \dot{x}}{\partial p_x} & 0 \\ 0 & 0 & 0 & \frac{\partial \dot{y}}{\partial p_y} \\ \frac{\partial \dot{p}_x}{\partial x} & \frac{\partial \dot{p}_x}{\partial y} & 0 & 0 \\ \frac{\partial \dot{p}_y}{\partial x} & \frac{\partial \dot{p}_y}{\partial y} & 0 & 0 \end{pmatrix} \quad (14)$$

For a point lying in a periodic orbit, $\mathbf{x}(T_p) - \mathbf{x}_0 = 0$, where $\mathbf{x} = (x, y, p_x, p_y)$ is a 4-dimensional phase space vector in our case and T_p is the period of the orbit.

We can define a function $F^p(x) = \mathbf{x}(T_p) - \mathbf{x}_0 = 0$. So that finding fixed points reduces to finding the roots of this function $F^p(x)$.

For an initial guess $\mathbf{x}_0$ that is near a fixed point, we can write function $F^{T_p}(x)$ as

$$F^{T_p}(\mathbf{x}_0) + DF^{T_p}(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) + \frac{\partial F^{T_p}(\mathbf{x})}{\partial t}(T - T_p) \;=\; 0 \quad (15)$$
$$F^{T_p}(\mathbf{x}_0) + (\mathbb{J}_p - \mathbb{I})(\mathbf{x} - \mathbf{x}_0) + \mathbf{v}(\mathbf{x})(T - T_p) \;=\; 0 \quad (16)$$

where $\mathbb{I}$ stands for the unit matrix. The jacobian, as we said before, satisfies the equation $\dot{\mathbb{J}} = \mathbb{A}\mathbb{J}$, where $A_{ij} = \frac{\partial v_i(x)}{\partial x_j}$

The condition for the Poincare section $g(\mathbf{x}) = 0$ expanded around the inital guess takes the form

$$g(\mathbf{x}_0) + \nabla g^{T_p}(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) \;=\; 0 \quad (17)$$
$$\mathbf{a}(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) \;=\; 0 \quad (18)$$

as $g(\mathbf{x}_0) = 0$ in the Poincare section. $\nabla g(\mathbf{x}) = \mathbf{a}$ is a vector in phase space perpendicular to the Poincare section. For each of our four Poincare sections, this vector is

$$\begin{aligned} a_{p_x+-} &= [0, 0, -1, 0] \\ a_{p_x-+} &= [0, 0, 1, 0] \\ a_{p_y+-} &= [0, 0, 0, -1] \\ a_{p_y-+} &= [0, 0, 0, 1] \end{aligned} \quad (19)$$

Since this is a Hamiltonian flow, energy must be conserved, $\mathbb{H} - E = 0$. This equation can be expanded around $\mathbf{x}_0$:

$$\mathbb{H}(\mathbf{x}_0) - E_0 + \nabla\mathbb{H}(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) - \mathbb{I}(E - E_p) \;=\; 0 \quad (20)$$
$$\nabla\mathbb{H}(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) - \mathbb{I}(E - E_p) \;=\; 0 \quad (21)$$

where $\nabla\mathbb{H}(\mathbf{x}_0)$ is given by

$$\nabla\mathbb{H} = \begin{pmatrix} -\dot{p_x} \\ -\dot{p_y} \\ \dot{x} \\ \dot{y} \end{pmatrix} = \begin{pmatrix} 8x(x^2-1)^3 + 2xy^2 \\ 2yx^2 + 2x\mu \\ p_x/m \\ p_y/m \end{pmatrix} \quad (22)$$

For finding periodic orbits of Hamiltonian flows, Cvitanovich suggests solving the system of equations

$$\begin{pmatrix} \mathbf{x}(T_0)-\mathbf{x}_0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} \mathbb{J}(\mathbf{x}_0)_p - \mathbb{I} & \mathbf{v}(\mathbf{x_0}) & 0 \\ \nabla g(\mathbf{x}_0) & 0 & 0 \\ \nabla \mathbb{H}(\mathbf{x}_0) & 0 & -\mathbb{I} \end{pmatrix} \begin{pmatrix} \mathbf{x}-\mathbf{x}_0 \\ T-T_0 \\ E-E_0 \end{pmatrix} = 0 \tag{23}$$

D. Numerical implementation

We used an eighth order Runge-Kutta integrator to integrate the system of differential equations containing d Hamilton's equations of motion 6 and $d \times d$ evolution equations for the Jacobian ??dej), for a total of $2d \times 2d$ system of differential equations. The integration stops when the trajectory hits a Poincare section. The Poincare section rutine employs interval splitting to land on the Poincare section. Although not very efficient, it is straightforward and it is our first approach to landing on the Poincare sections.

There are two main methods, among others, for finding periodic orbits. To use a single-shooting root-finding rutine, one guesses an initial point on a Poincare section and the rutine searches for a nearby point whose evolution is the same point. This requires very good guesses and in our case the highly chaotic motion in the double well doesn't allow it.

Multi-shooting root-finding is a method for which one gives n guesses to search for an orbit of period n. In our case, if we are looking for cycle $\overline{RULD}$, we should start with one point on each Poincare section. Multi-shooting allows us to look for specific cycles that the symbolic dynamics suggests.

We implemented this rutine but it was time consuming because it must take into account each of the Poincare sections, the conservation of energy, equations for Jacobian and equations of motion for the trajectories. He had trouble with the conservation of energy while using the system of equations suggested by Cvitanovic in ??. We realized that even though the initial guess lied in e certain energy shell, that didn't imply that the multishooting rutine would evolve into a point with the same energy. So we decided to review the original equations for deriving the matrix in Eq. 23. We found that the term $\mathbb{H}(\mathbf{x}_0) - E_0$ of Eq. 21 should not be dropped because it ensures that the following points in the rutine lie in the correct erengy shell.

The system of equations that we finally solved was the matrix of Eq. 23 but with $H(x) - E_0$ beneath $\mathbf{x}(T_0) - \mathbf{x}_0$. Including this term fixed the energy of the evolving points of the mutlishooting rutine.

III. DISCUSSION

The ultimate goals of the project was to learn about the dynamics in the double well calculating the diffusion and to compute the diffusion coefficient for a particle in the double well, if time allowed. But this last part was not achieved because we couldn't find non-trivial periodic orbits for this system (by trivial, I refer to the horizontal and vertical cycles). There were several things that slowed the work. The highly chaotic motion of the particles made it extremely difficult to even guess what cycles could exist. To do this we computed the trajectories for different initial points on the horizontal and vertical axis to gain some insight into the dynamics of the system. The only trajectory resembling a cycle, besides the trivial ones, is plotted in Fig. ??. This only suggested that we should modify our symbolic dynamics and left us a sense of doubt about the symbols we choose, because we couldn't know if a strange cycles could appear that where not uniquely defined by our symbolic dynamics. We struggled between choosing single-shooting or multi-shooting. The former was simpler to implement but we had no warranty that we where going to find all the small cycles because you only give a guess and hope for the rutine to find a cycle nearby, any cycle, and since the accuracy of period orbit theory depends on the shortest cycle left out we were not sure of this method. Multishooting appeared more efficient in that respect, we could search for cycles corresponding to the words given by our symbolic dynamics. But it required more programming and the initial guesses should be choosen wisely or the multishooting program doesn't converge quickly. The multishooting gueeses have to be computed in another programm that gives us initial points on different Poncare sections. The inconvenient with mutlishooting is that it appears to be time consuming to find cycles for this system. For a cycle of period 5, the root solving rutine should solve a 30×30 system of equations and integrate a system of 20 differential equations at every step. Even though our multishooting rutine apparently worked fine, $f(x) - x$ appears to converged to zero, it evolved to slow for us to find any period orbit.

I attained the minimal goal of learning about periodic orbit theory and how to use symbolic dynamics to describe a system. I will modify my rutine for hitting the Poincare section to see if this speeds up the calculations, because I still want to find periodic orbits for this system even if they are very simple.

The main result is implementing a program that employs multishooting to find periodic orbits for n-dimensional Hamiltonian flows with m-Poincare sections and including the term $H(x) - E_0$ to ensure energy is conserved. Due to shortage of time, this programm could not be fully proved.

Acknowledgments

I would like to thank Prof. Cvitanovic for teaching me about Chaos and how periodic orbit theory can be used to study the dynamics of chaotic systems. I also want to thank Slaven Peleš for all his suggestions throught this research. Last but not least, I want to thank Jorge Millan for useful discussions on the subject.

APPENDIX A: PROJECT PLAN

Schedule of which part I intend to deliver by which date:

1. **Thu Oct 23:** Write the Hamilton's equations of motion, and the equations of variations for the system. Integration of system of equations to obtain trajectories projected onto the configuration space, and in the phase space .

2. **Thu Oct 30:** Define a Poincare section. Plot typical trajectories in the Poincare section.

3. **Thu Nov 06:** Attempt to construct a symbolic dynamics. Write a program to find periodic orbits.

4. **Thu Nov 13:** Continue determinig the shortest cycles.

5. **Thu Nov 20:** Calculate stability and period of periodic cycles

6. **Thu Nov 27:** Generate spectral determinant expansion in terms of pseudocycles.

7. **Thu Dec 04:** Calculate diffusion coefficient.Discuss qualitatively the dependence on the parameter μ.

8. **Thu Dec 11:** Project deadline

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