

UPOsHam: A Python package for computing unstable periodic orbits in two degrees of freedom Hamiltonian systems

January 7, 2020

Statement of Need

Hamiltonian systems model a diverse array of problems in physical sciences and engineering. In Hamiltonian systems the fundamental phase space structure that partitions dynamically distinct trajectories and mediates transition between multi-stable regions are **stable** and **unstable invariant manifold**. In a $2N$ dimensional Hamiltonian phase space, the invariant manifold has 2 less dimension than the phase space and is anchored to the **normally hyperbolic invariant manifold** (NHIM) which has 3 less dimension. For 2 degrees of freedom or four dimensional phase space, the NHIM is an **unstable periodic orbit** (UPO) around the index-1 saddle equilibrium point (Wiggins 2016). Since in this case, the UPO anchors the invariant manifolds that partition trajectories, their computation and stability analysis forms the starting point for dynamical systems analysis. UPOsHam is meant to serve this purpose by providing a module of numerical methods, along with example Hamiltonian systems, for computing the unstable periodic orbits (UPOs) at any specified total energy as long as their existence is guaranteed. Even though, there are existing numerical methods for computing UPOs, we have found that they either lack in reproducibility, or have steep learning curve for using the software, or have been written using closed source software, and at times combination of these (Farantos 1998; Pollak, Child, and Pechukas 1980). Our aim is to provide an open source package that implements some of the standard methods and shows the results in the context of example Hamiltonian systems. This is meant as a starting point to integrate other numerical methods in an open source package such that UPOs computed in dynamical systems papers can be reproduced with minimal tweaking while providing an exploratory environment to further develop the underlying methods.

Summary

The Python package, UPOsHam, is a collection of three methods in the form of submodules under `uposham` for computing unstable periodic orbits around index-1 saddles in the bottleneck of Hamiltonian systems. When the form is kinetic (purely momenta dependent terms) plus potential energy, the unstable periodic orbits project as lines on the configuration space (x, y) and connect opposite points of an equipotential line $V(x, y) = E$. The three methods described below have been implemented for example Hamiltonian systems (also available as submodules under `uposham`) and are described in §:Examples. The demonstration scripts available in the package show how to import each of the methods and implement system specific functions for computing the unstable periodic orbit.

The computed unstable periodic orbits using the three methods for the coupled quartic Hamiltonian are compared in Figure 1.

Features: Available Methods

In this package, the user has the option to choose between the three methods described below. These are implemented in separate scripts with functions that can be modified to define the total energy (Hamiltonian), potential energy, vector field, Jacobian, variational equations (Parker and Chua 1989).

Turning point

This method is based on finding the UPO by detecting trajectories initialized on the equipotential contour ($V(x, y) = E$ where $V(x, y)$ is the potential energy function and E is the total energy) that turn in the opposite directions (Pollak, Child, and Pechukas 1980). This method relies on the fact that for Hamiltonians of the form kinetic plus potential energy the UPO is the limiting trajectory that bounces back and forth between the equipotential contour corresponding to the given total energy. So to converge on this limiting trajectory, the turning point method iteratively decreases the gap between the bounding trajectories that turn in the opposite directions. Detection of turning is done using a dot product condition which leads to stalling of the method beyond a certain tolerance (typically 10^{-6} in the examples here.)

Turning point based on configuration difference

Based on the turning point approach, we have implemented a **new method** which shows stable convergence and does not rely on the dot product formula. Suppose we have found two initial conditions on a given equipotential contour and they turn in the opposite directions. If the difference in x -coordinates is small ($\approx 10^{-2}$), the generated trajectories will approach the UPO from either sides. If the difference in x -coordinates is large, we can integrate the Hamilton's equations for a guess time interval and find the turning point (event using ODE event detection) at which the trajectories bounce back from the far side of the equipotential contour in opposite directions. We choose these two points as our initial guess and the difference of x -coordinates become small now. Without loss of generality, this method can be modified to either pick the difference of y -coordinates or a combination of x and y coordinates. This choice will depend on the orientation of the potential energy surface's bottleneck in the configuration space.

Differential correction

This method is based on small ($\approx 10^{-5}$) corrections to the initial conditions of an UPO and continuing to desired total energy. The procedure is started from the linear solutions of the Hamilton's equations and which generates a small amplitude ($\approx 10^{-5}$) UPO. This is fed into the procedure that calculates correction to the initial condition based on error in the terminal condition of the UPO. This leads to convergence within 3 steps in the sense of the trajectory returning to the initial condition. Once a small amplitude UPO is obtained, numerical continuation increases the amplitude and correspondingly total energy, while a combination of bracketing and bisection method computes the UPO at the desired energy for a specified tolerance (Naik and Wiggins 2019; Koon et al. 2011).

Examples

Consider the following two degrees-of-freedom Hamiltonian model where x, y are configuration space coordinates and p_x, p_y are corresponding momenta, $V(x, y)$ is the potential energy, and $T(x, y)$ is the kinetic energy.

Quartic Hamiltonian

This Hamiltonian can be considered as a low dimensional model of a *reaction* in a bath where the coupling is controlled using a parameter. The potential energy is a double-well surface and the bath is modeled using a harmonic oscillator.

$$\mathcal{H}(x, y, p_x, p_y) = \frac{p_x^2}{2} - \alpha \frac{x^2}{2} + \beta \frac{x^4}{4} + \frac{\omega}{2} (p_y^2 + y^2) + \frac{\epsilon}{2} (x - y)^2 \quad (1)$$

where $\alpha, \beta, \omega, \epsilon$ are free parameters. When $\epsilon \neq 0$, the system is referred to as the *coupled quartic Hamiltonian*, and *uncoupled quartic Hamiltonian* otherwise.

De Leon-Berne Hamiltonian

This Hamiltonian has been studied as a model of isomerization of a single molecule that undergoes conformational change (De Leon and Berne 1981; De Leon and Marston 1989) and exhibits regular and chaotic dynamics relevant for chemical reactions.

$$\mathcal{H}(x, y, p_x, p_y) = T(p_x, p_y) + V_{\text{DB}}(x, y) = \frac{p_x^2}{2m_A} + \frac{p_y^2}{2m_B} + V_{\text{DB}}(x, y) \quad (2)$$

where the potential energy function $V_{\text{DB}}(x, y)$ is

$$\begin{aligned} V_{\text{DB}}(x, y) &= V(x) + V(y) + V(x, y) \\ V(y) &= 4y^2(y^2 - 1) + \epsilon_s \\ V(x) &= D_x [1 - \exp(-\lambda x)]^2 \\ V(x, y) &= 4y^2(y^2 - 1) [\exp(-\zeta \lambda x) - 1] \end{aligned} \quad (3)$$

The parameters in the model are m_A, m_B which represent mass of the isomers, while ϵ_s, D_x denote the energy of the saddle, dissociation energy of the Morse oscillator, respectively, and will be kept fixed in this study, λ, ζ denote the range of the Morse oscillator and coupling parameter between the x and y configuration space coordinates, respectively.

Visualization: Unstable periodic orbits

Relation to ongoing research projects

We are developing geometric methods of phase space transport in the context of chemical reaction dynamics that rely on identifying and computing the unstable periodic orbits. Manuscripts related to the Quartic Hamiltonian and De Leon-Berne Hamiltonian is under preparation.

Acknowledgements

We acknowledge the support of EPSRC Grant No. EP/P021123/1 and Office of Naval Research (Grant No. N00014-01-1-0769). The authors would like to acknowledge the London Mathematical Society and School of Mathematics at the University of Bristol for supporting the undergraduate research bursary 2019. We acknowledge contributions from Shane Ross for the early MATLAB version of the differential correction and numerical continuation code.

References

- De Leon, N., and B. J. Berne. 1981. "Intramolecular Rate Process: Isomerization Dynamics and the Transition to Chaos." *The Journal of Chemical Physics* 75 (7): 3495–3510. doi:10.1063/1.442459.
- De Leon, N., and C. C. Marston. 1989. "Order in Chaos and the Dynamics and Kinetics of Unimolecular Conformational Isomerization." *The Journal of Chemical Physics* 91 (6): 3405–25. doi:10.1063/1.456915.
- Farantos, Stavros C. 1998. "POMULT: A Program for Computing Periodic Orbits in Hamiltonian Systems Based on Multiple Shooting Algorithms." *Computer Physics Communications* 108 (2-3). Elsevier: 240–58.

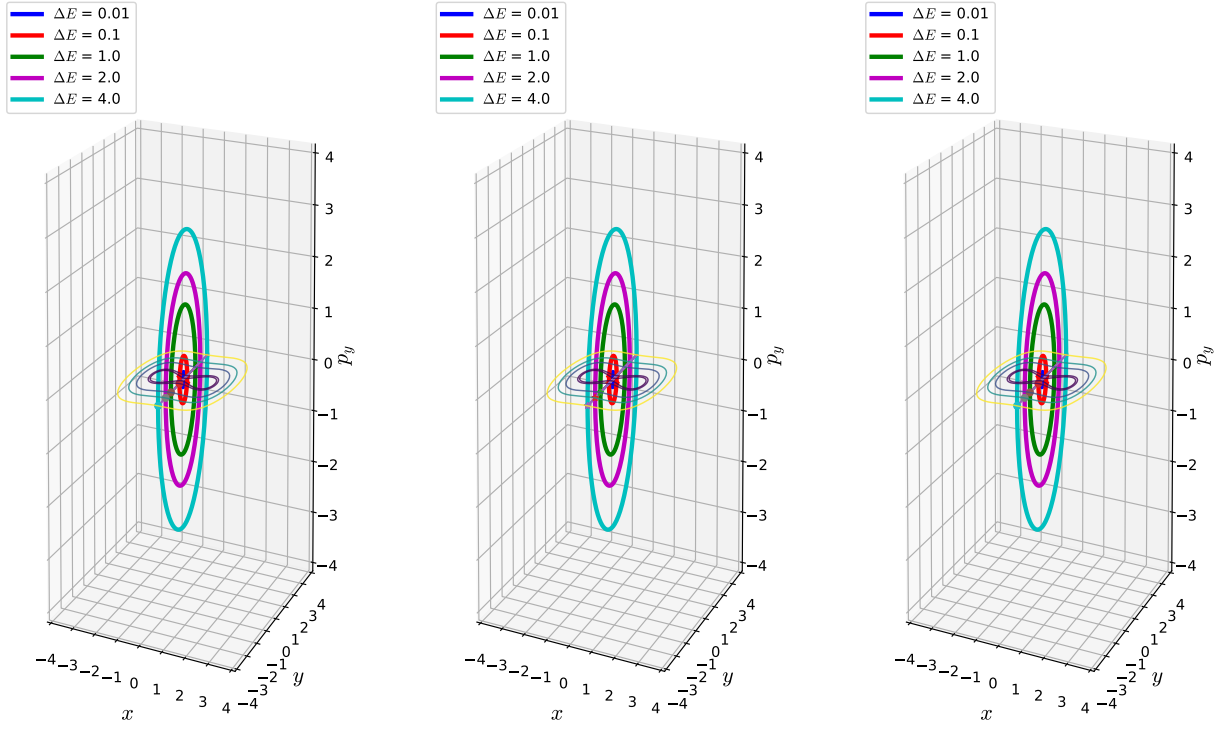


Figure 1: Comparing the turning point, turning point based on configuration difference, and differential correction methods for the coupled quartic Hamiltonian.

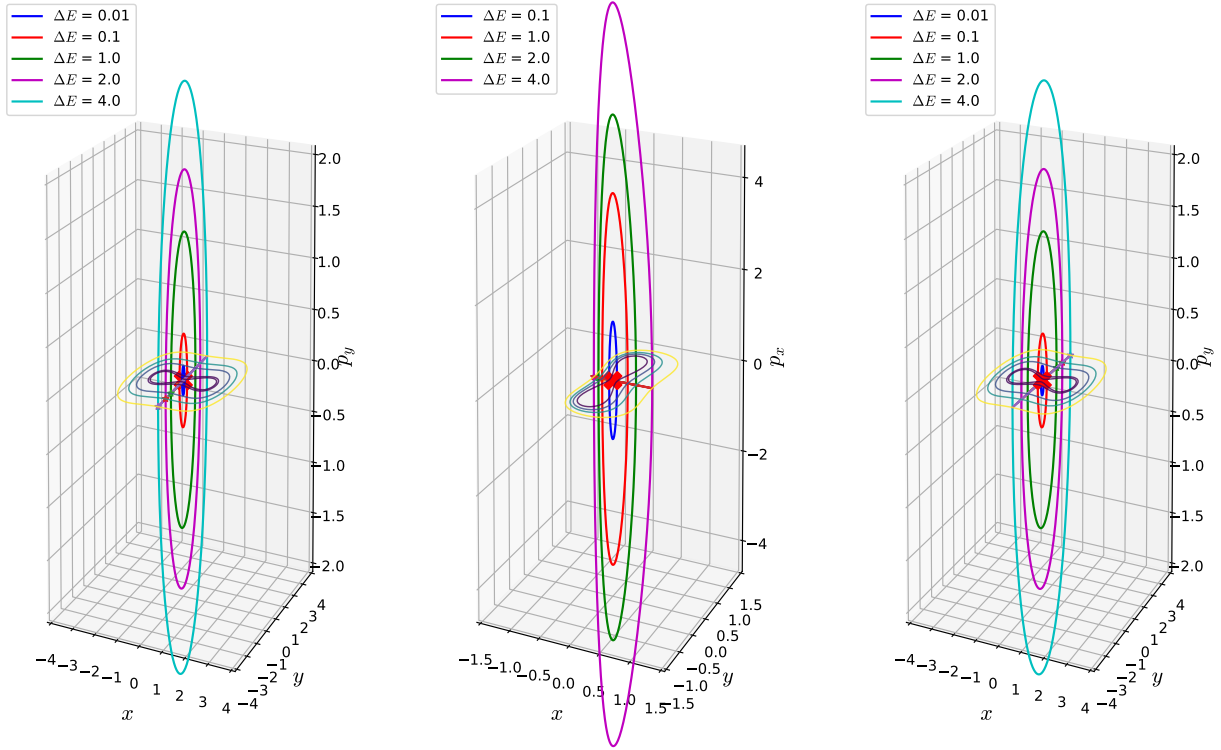


Figure 2: Comparing the turning point based on configuration difference method for the three Hamiltonians

doi:10.1016/S0010-4655(97)00131-8.

Koon, W. S., M. W. Lo, J. E. Marsden, and S. D. Ross. 2011. *Dynamical systems, the three-body problem and space mission design*. Marsden books. ISBN: 978-0-615-24095-4.

Naik, Shibabrat, and Stephen Wiggins. 2019. “Finding Normally Hyperbolic Invariant Manifolds in Two and Three Degrees of Freedom with Hénon-Heiles-Type Potential.” *Phys. Rev. E* 100 (2): 022204. doi:10.1103/PhysRevE.100.022204.

Parker, T. S., and L. O. Chua. 1989. *Practical Numerical Algorithms for Chaotic Systems*. New York, NY, USA: Springer-Verlag New York, Inc. ISBN: 0-387-96689-7.

Pollak, Eli, Mark S. Child, and Philip Pechukas. 1980. “Classical Transition State Theory: A Lower Bound to the Reaction Probability.” *The Journal of Chemical Physics* 72 (3): 1669–78. doi:10.1063/1.439276.

Wiggins, Stephen. 2016. “The Role of Normally Hyperbolic Invariant Manifolds (NHIMs) in the Context of the Phase Space Setting for Chemical Reaction Dynamics.” *Regular and Chaotic Dynamics* 21 (6): 621–38. doi:10.1134/S1560354716060034.