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

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Software repository

Statement of Need

In Hamiltonian systems the fundamental phase space structure that partitions dynamically disparate trajectories and mediates transition between multi-stable regions is an invariant manifold of 1 less dimension than the energy surface. In a 2N dimensional phase space, these invariant manifolds are anchored to the normally hyperbolic invariant manifold which becomes an unstable periodic orbit (UPO) in the four dimensional phase space (Wiggins 2016). Since the UPO forms the basis for distinguishing trajectories, their computation and stability analysis is the starting point for dynamical systems analysis. This Python package provides a collection of three methods for computing the unstable periodic orbits (UPOs) at any specified total energy as long as their existence is guaranteed. Even though, there is no lack of 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. Our aim is to provide an open source package that implements some of the standard methods and shows the results in the context of model problems. This is meant as an encouragement to integrate other successful methods into this package in a reproducible and less steep of a learning curve.

Summary

UPOsHam is a collection of three useful methods for computing unstable periodic orbits in Hamiltonian systems that model a diverse array of problems in physical sciences and engineering. The methods have been implemented for three example Hamiltonian systems that are prototypical models of chemical reactions.

We show few example computations of the unstable periodic orbit for these examples in Fig. 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 Hamiltonian total energy, potential energy, vector field, Jacobian, variational equations (Parker and Chua 1989).

Turning point

Hamiltonian systems of the form kinetic plus potential energy have unstable periodic orbits in the bottleneck that touches the equipotential lines given by $V(x, y) = E$. This method is based on finding the UPO by checking for trajectories that turn in the opposite directions and iteratively bringing them closer to approximate the UPO (Pollak, Child, and Pechukas 1980).

Differential turning point

Differential correction and numerical continuation

Examples

Consider the following two degrees-of-freedom Hamiltonian model of a reaction in a bath (solvent)

Uncoupled quartic Hamiltonian

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

Coupled quartic Hamiltonian

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

DeLeon-Berne Hamiltonian

This Hamiltonian has been studied in chemical reaction dynamics as a model of isomerization of a single molecule that undergoes structural changes (Nelson De Leon and Berne 1981; N De Leon and Marston 1989). This model Hamiltonian exhibits chaotic dynamics when the coupling between the double well and Morse oscillator is increased.

$$\mathcal{H}(x, y, p_x, p_y) = T(p_x, p_y) + V_{\mathrm{DB}}(x, y) = \frac{p_x^2}{2m_A} + \frac{p_y^2}{2m_B} + V_{\mathrm{DB}}(x, y) \tag{3}$$

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

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

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 in the bottleneck

Relation to ongoing research projects

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

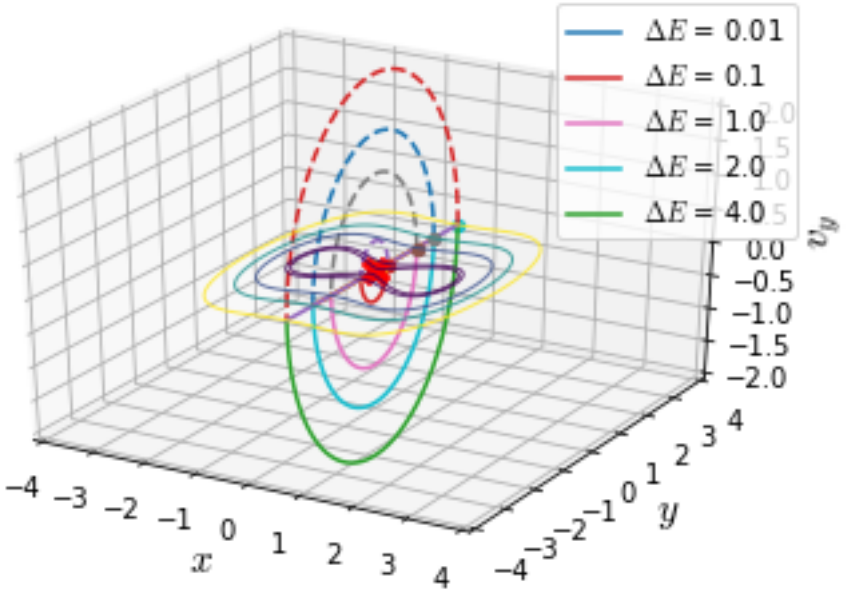

Figure 1: Uncoupled system

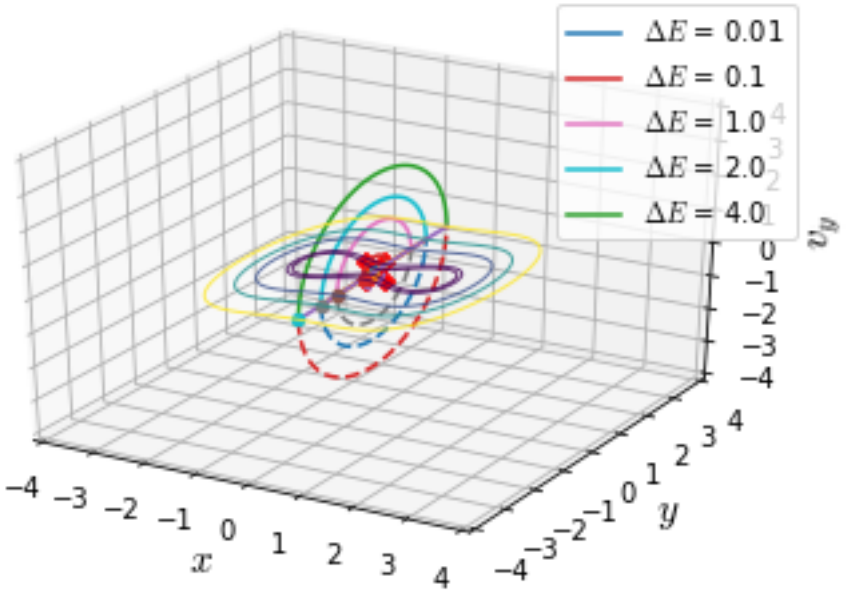

Figure 2: Coupled system

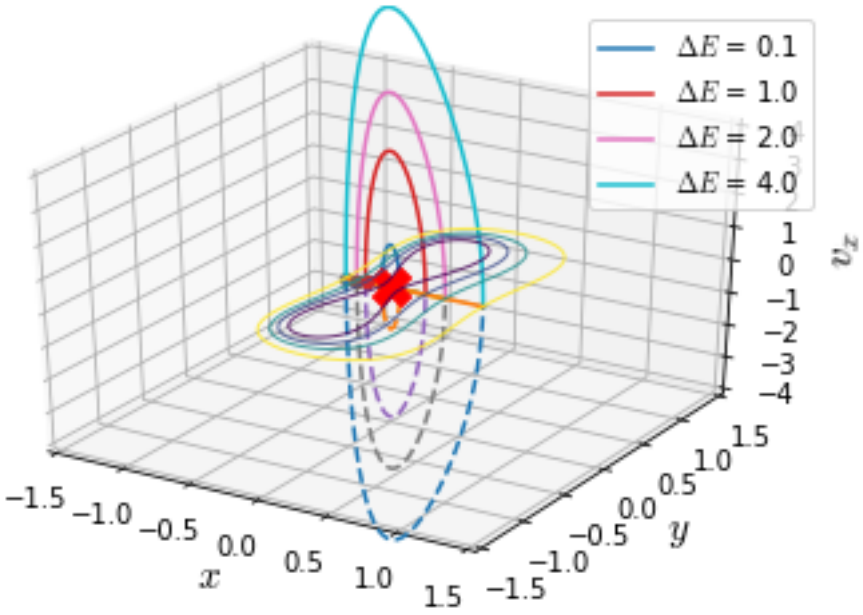

Figure 3: De Leon-Berne system

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