UPOsHam

Contents

Summary

This Python package is a collection of three methods for computing unstable periodic orbits in two degrees of freedom Hamiltonian systems that model a diverse array of problems in physical sciences and engineering (Parker and Chua 1989; Wiggins 2003). The unstable periodic orbits exist in the bottleneck of the equipotential line $V(x, y) = E$ and project as lines on the configuration space (x, y) for the Hamiltonian system of the form kinetic plus potential energy (Wiggins 2016). The three methods implemented here (and available under src directory) has been used in (Pollak, Child, and Pechukas 1980; De Leon and Berne 1981; Wang Sang Koon et al. 2000; W. S. Koon et al. 2011; Naik and Ross 2017; Ross et al. 2018; Naik and Wiggins 2019) for transition dynamics in chemical reactions, celestial mechanics, and ship capsize. We have chosen three Hamiltonian systems that have two wells connected by a bottleneck where the unstable periodic orbits exist for energy above the energy of the saddle equilibrium point. A brief description of these systems can be found in the paper.

Installation

Clone/download the git repository using

```
$ git clone git@github.com:WyLyu/UPOsHam.git
$ cd UPOsHam
$ pip install -r requirements.txt (or pip3 install -r requirements.txt)
```

and check the modules shown in requirements.txt are installed using conda/pip.

Usage

The example scripts that computes the unstable periodic orbits (UPOs) for a given Hamiltonian system is in the examples directory with names `<method>_<system>.py`. For example, to compute the unstable periodic orbits (the default shows at 2 total energy levels) for the De Leon-Berne Hamiltonian (1981) using the differential correction method can be run from the command line by calling

```
$ python examples/differential_correction_deleonberne.py
```

This will save data files in the current directory and save the following plot in the plots directory.

Fig. Unstable periodic orbits for De Leon-Berne Hamiltonian

The example scripts import the system specific functions and method specific functions to obtain the UPOs. These are written as illustration of how to apply these methods to new systems.

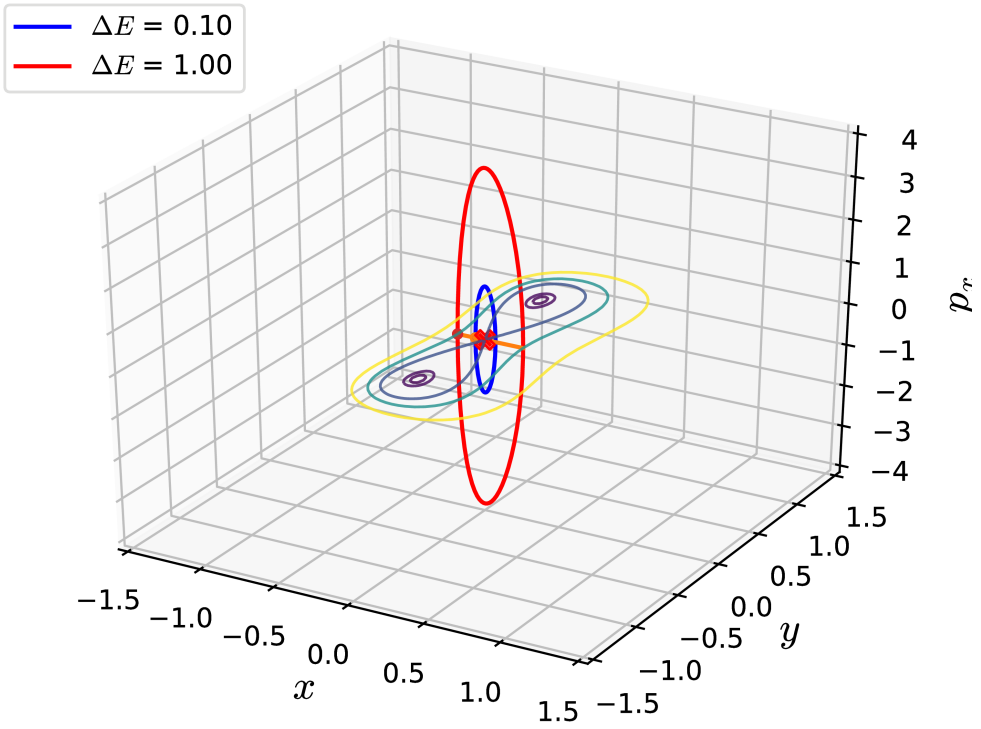

Figure 1:

Comparing the methods for the coupled quartic Hamiltonian

We demonstrate how the UPOs computed using the different methods compare with each other for a specific system: coupled quartic Hamiltonian.

Comparison of the results (data is located here) obtained using the three methods for the coupled quartic Hamiltonian can be done using

```
$ ipython
>>> run ./tests/compare_methods_coupled.py
```

and the generated figure is located here

To obtain the unstable periodic orbits for a specific model Hamiltonian using a specific method, one uses

```
$ ipython
>>> run ./examples/diffcorr_UPOs_coupled.py
```

Other tests can be performed by running the cells in the ./tests/tests.ipynb

Contributing

Guidelines on how to contribute to this package can be found here along with the code of conduct here for engaging with the fellow contributors.

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