Origin fate map: a simple and efficient numerical tool for analyzing phase space transport

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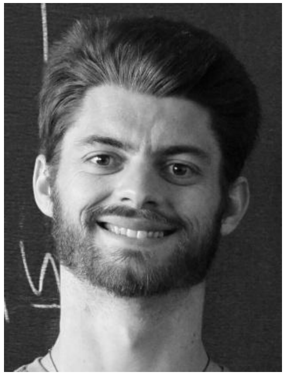
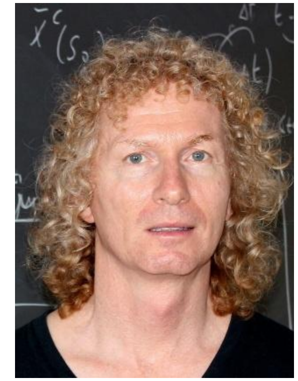
Work in collaboration with





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Navigating phase space transport with the origin-fate map

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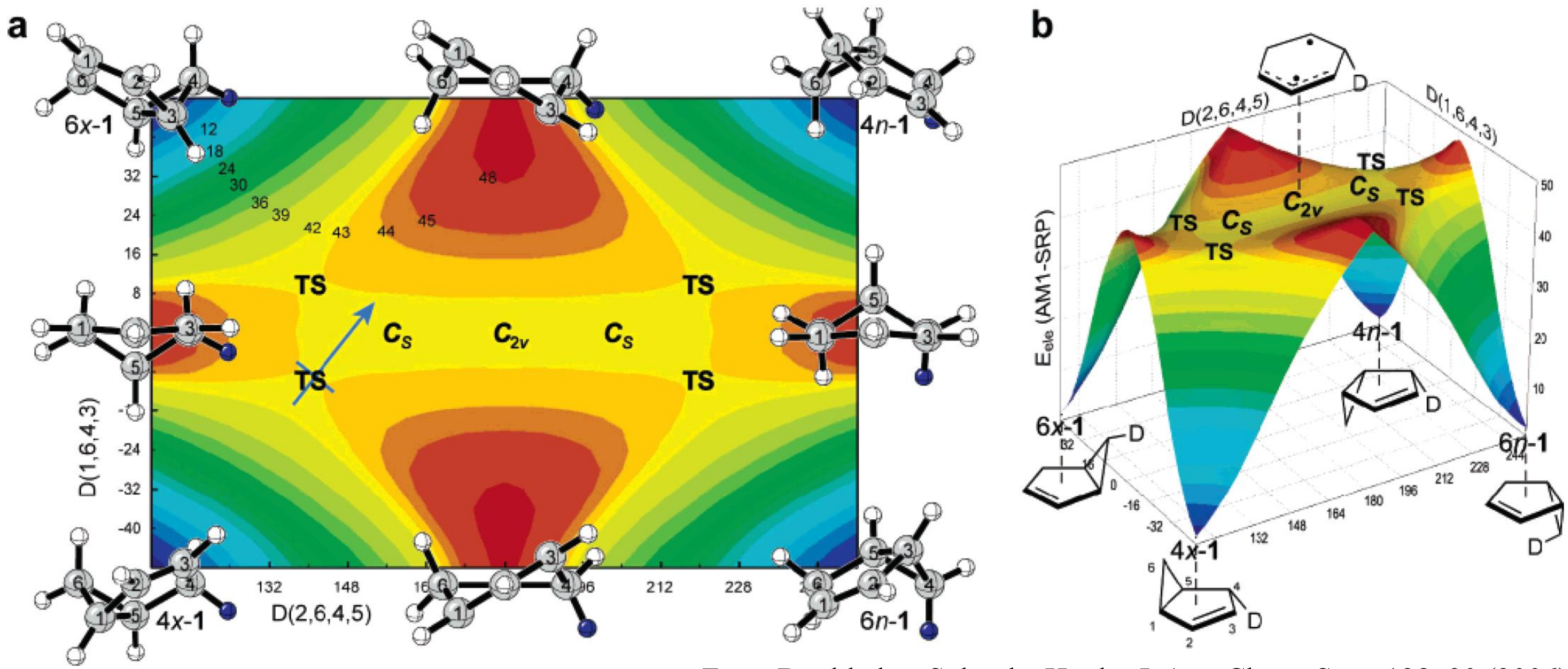
Outline

- The 2 degree of freedom caldera Hamiltonian system
- The origin fate map (OFM)
  - ✓ Definition
  - ✓ Visualization of phase space transport
  - ✓ Relation to the morphology of manifolds
    - Lagrangian descriptors
  - ✓ Locating the position of unstable periodic orbits
- Summary

The caldera potential energy surface

Caldera type potentials, having a potential energy plateau, describe organic chemistry reactions.



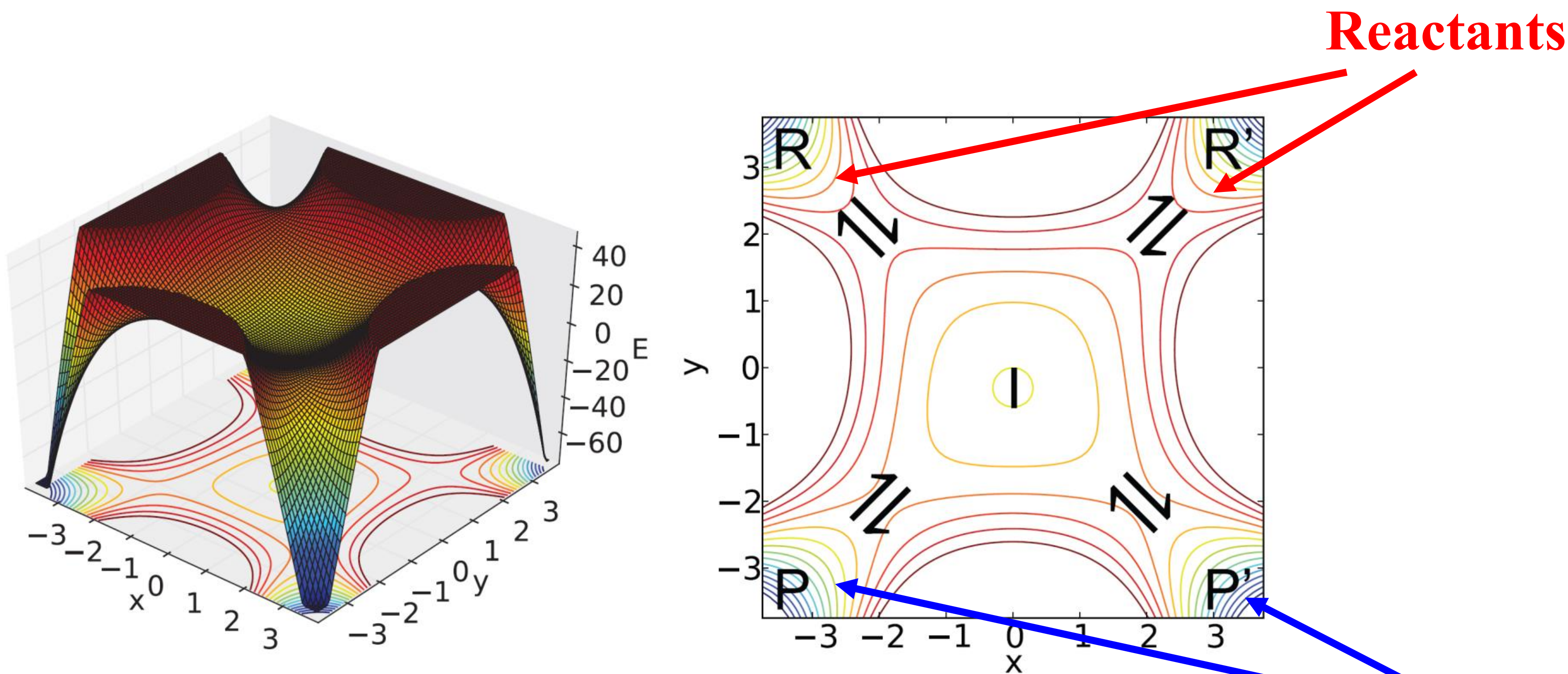
From Doubleday, Suhrada, Houk., J. Am. Chem. Soc., 128, 90 (2006)

The so-called AM1-SRP potential has 32 parameters, obtained through fittings with experimental and simulation data, describes different pathways from a single reactant to three products (Doubleday et al., J. Am. Chem. Soc., 2006).

The caldera potential energy surface

Caldera potential: a shallow potential well with two pairs of symmetry related index-1 saddles associated with entrance/exit channels.

Index-1 saddle: a critical point of the potential corresponding to a local minimum in one direction and a local maximum in another.



From Collins, Kramer, Carpenter, Ezra, Wiggins, J. Chem. Phys., 141, 034111 (2014)

The caldera Hamiltonian system

We consider the 2 degree of freedom Hamiltonian system (Collins et al., J. Chem. Phys., 2014 - Katsanikas, Wiggins, Int. J. Bifurcat. Chaos, 2018; 2019 - Katsanikas et al., Int. J. Bifurcat. Chaos, 2020; Chem. Phys. Lett., 2020):

$$H(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) + V(x, y)$$

where

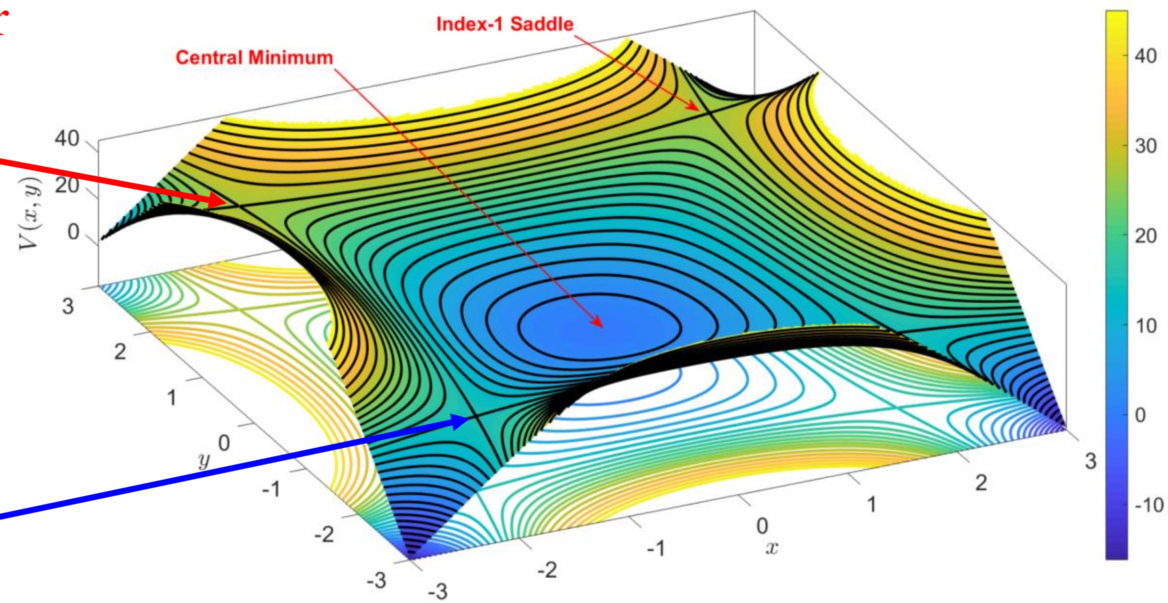
$$V(x, y) = c_1[(\lambda x)^2 + y^2] + c_2 y - c_3[(\lambda x)^4 + y^4 - 6(\lambda x)^2 y^2],$$

with $c_1 = 5, c_2 = 3, c_3 = -0.3$, $E = H(x, y, p_x, p_y)$ is the system's energy and λ being a 'stretching' parameter

E=27.0123

Symmetric potential: λ=1

E=14.767

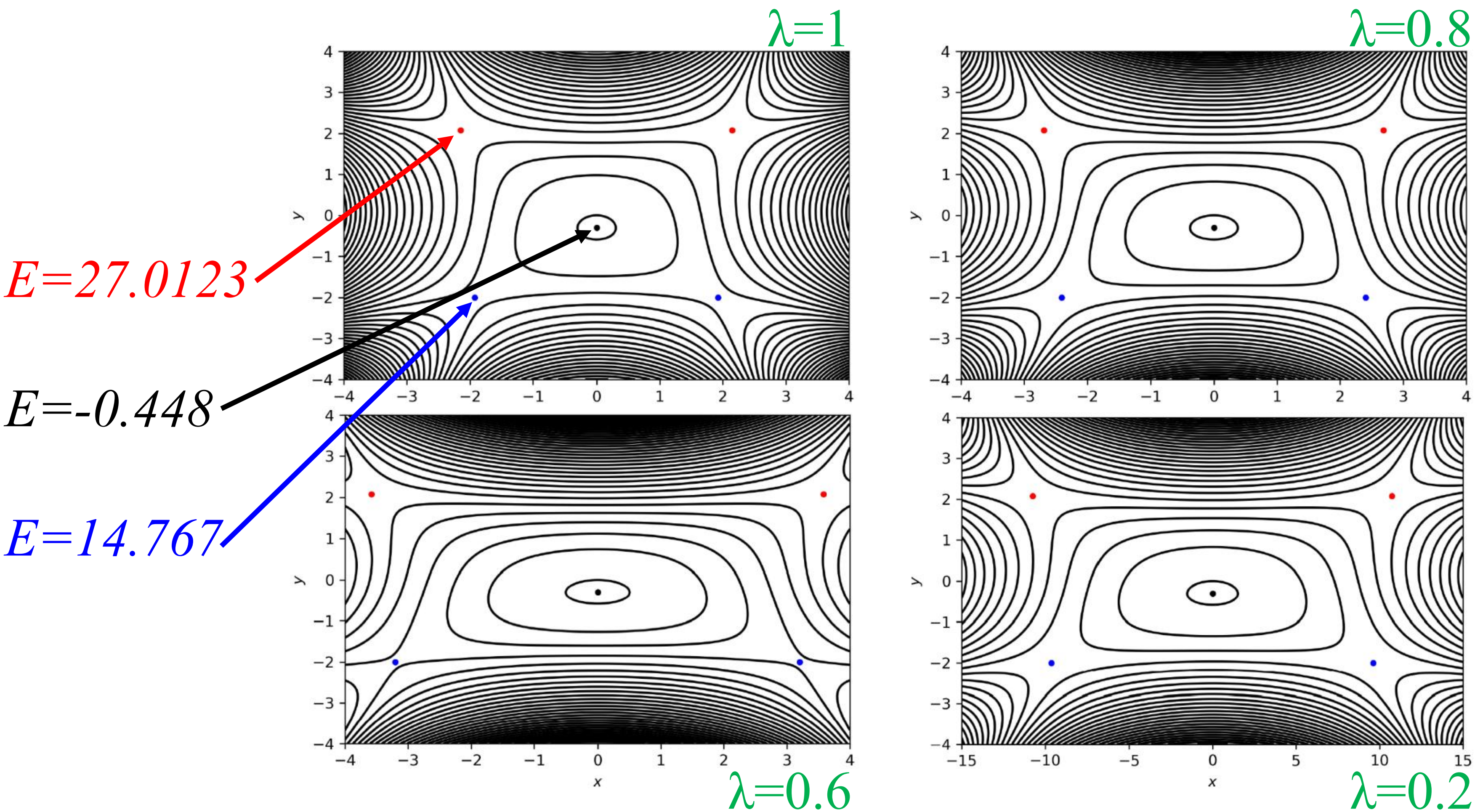


From Katsanikas, García-Garrido, Wiggins, Int. J. Bifurcat. Chaos, 30, 2030026 (2020)

The caldera Hamiltonian system

$$V(x,y) = c_1[(\lambda x)^2 + y^2] + c_2 y - c_3[(\lambda x)^4 + y^4 - 6(\lambda x)^2 y^2]$$

Stretched potential (typically, $0 < \lambda < 1$)



From Katsanikas, Wiggins, Int. J. Bifurcat. Chaos, 29, 1950057 (2019)

Dynamical matching

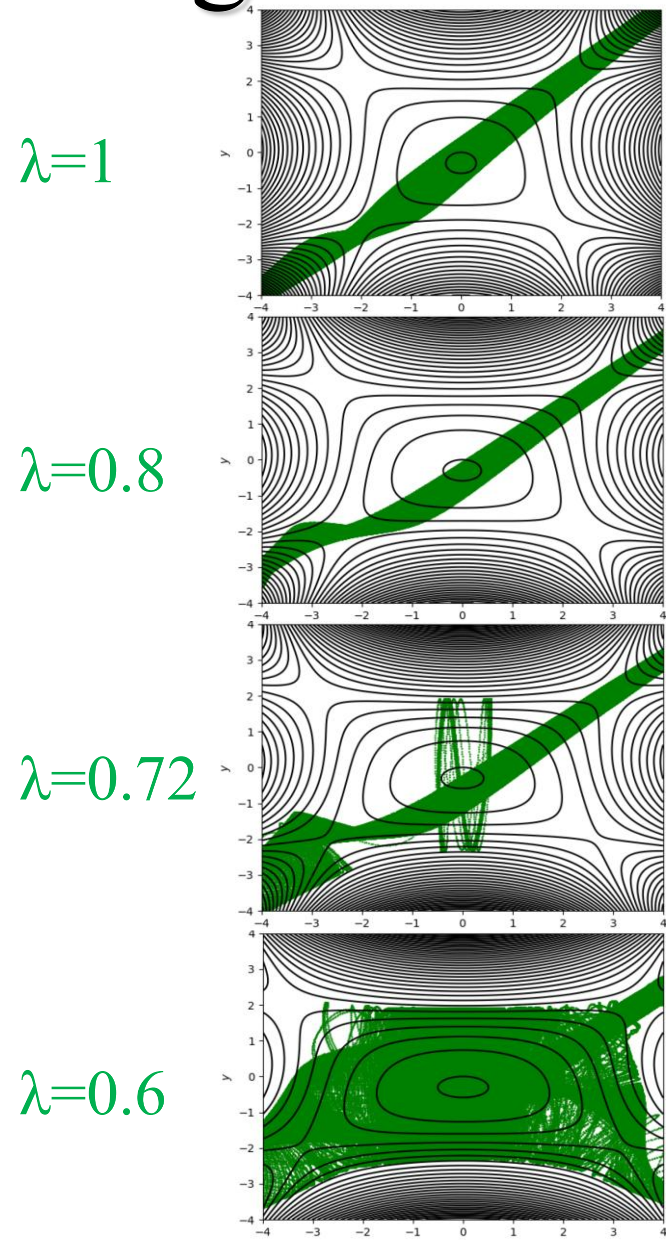
Dynamical matching: the momentum direction associated with an incoming orbit initiated at a high energy saddle point, practically determines the outcome of the reaction, i.e. the orbit passes through the diametrically opposing exit channel.

Critical value for the breaking of dynamical matching: $\lambda = 0.778$ (Katsanikas et al., Int. J. Bifurcat. Chaos, 2020)

The unstable manifolds of the unstable periodic orbits of the upper saddles

start interacting with

the stable manifolds of the central area unstable periodic orbits.



From Katsanikas, Wiggins, Int. J. Bifurcat. Chaos, 28, 1830042 (2018) and 29, 1950057 (2019)

The origin fate map (OFM)

Origin fate map (OFM): We assign to sets of initial conditions a particular combination of indices indicating their origin or start state (through backward integration) and their fate or end state (via forward integration).

Symmetric potential: $\lambda=1$

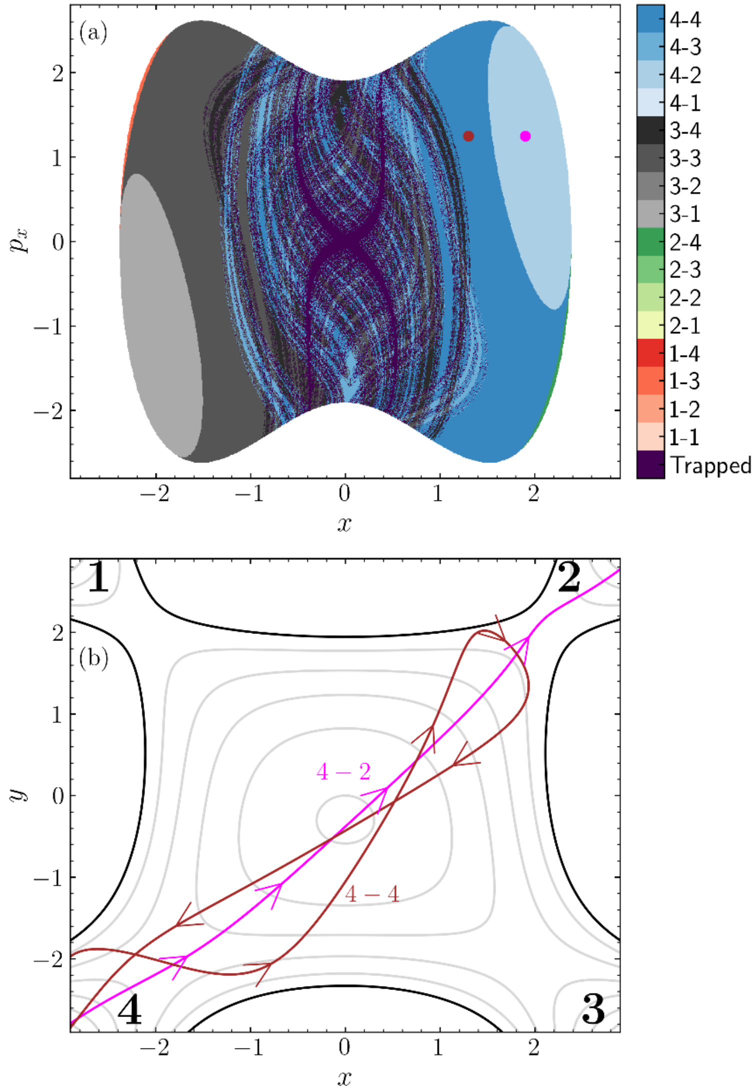
Poincaré surface of section (PSS):

$$y = 1.88409, \qquad p_y > 0,$$
$$E = 29.$$

Integration time: $\tau = 20$ time units.

Escape condition: $|y| > 6$

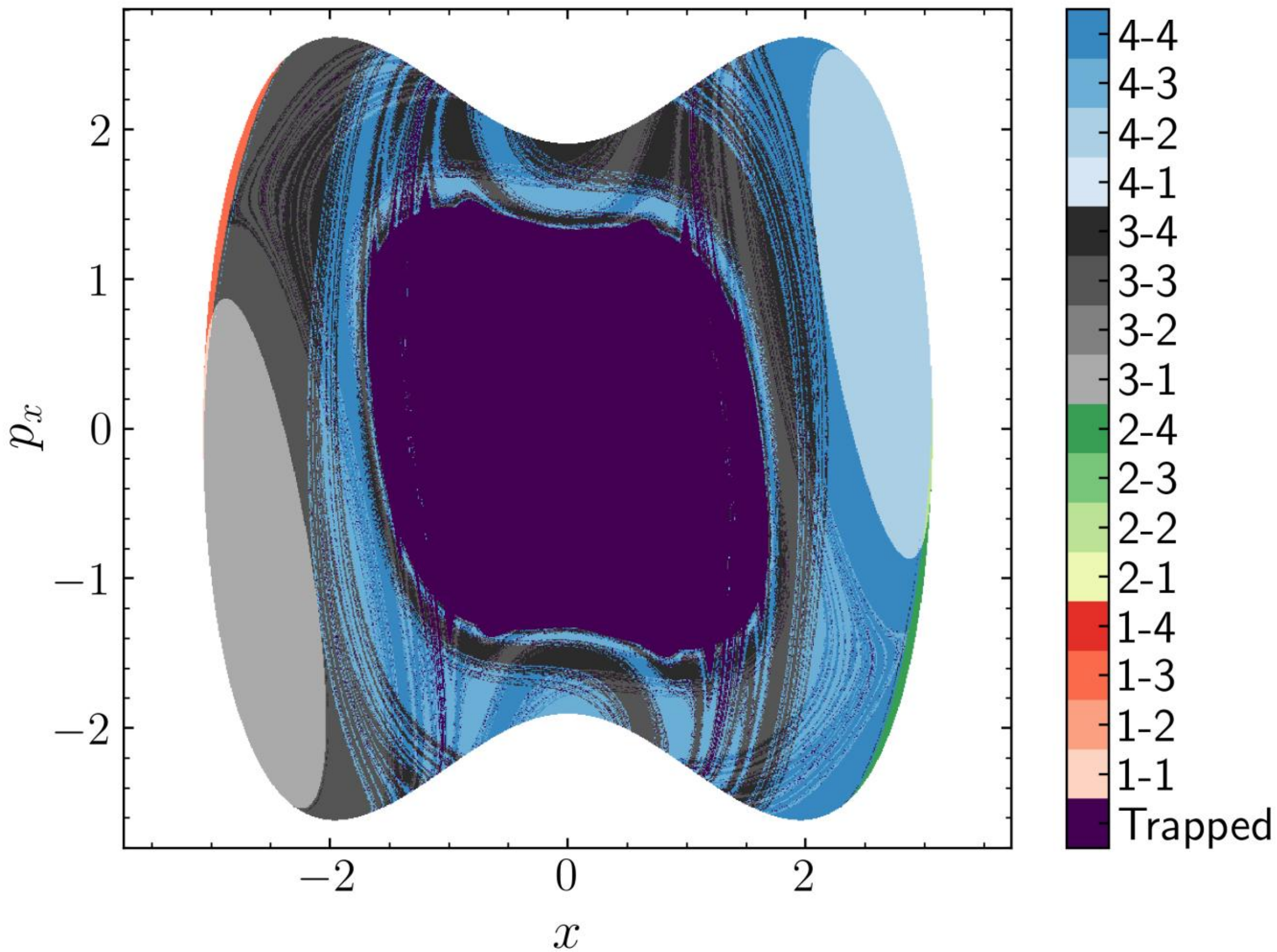
Trapped: an orbit does not escape in either the forward or backward integration.



The origin fate map (OFM)

Stretched potential: λ=0.778

PSS: $y = 1.88409,\ p_y > 0, E = 29$. Integration time: $\tau = 20$ time units.

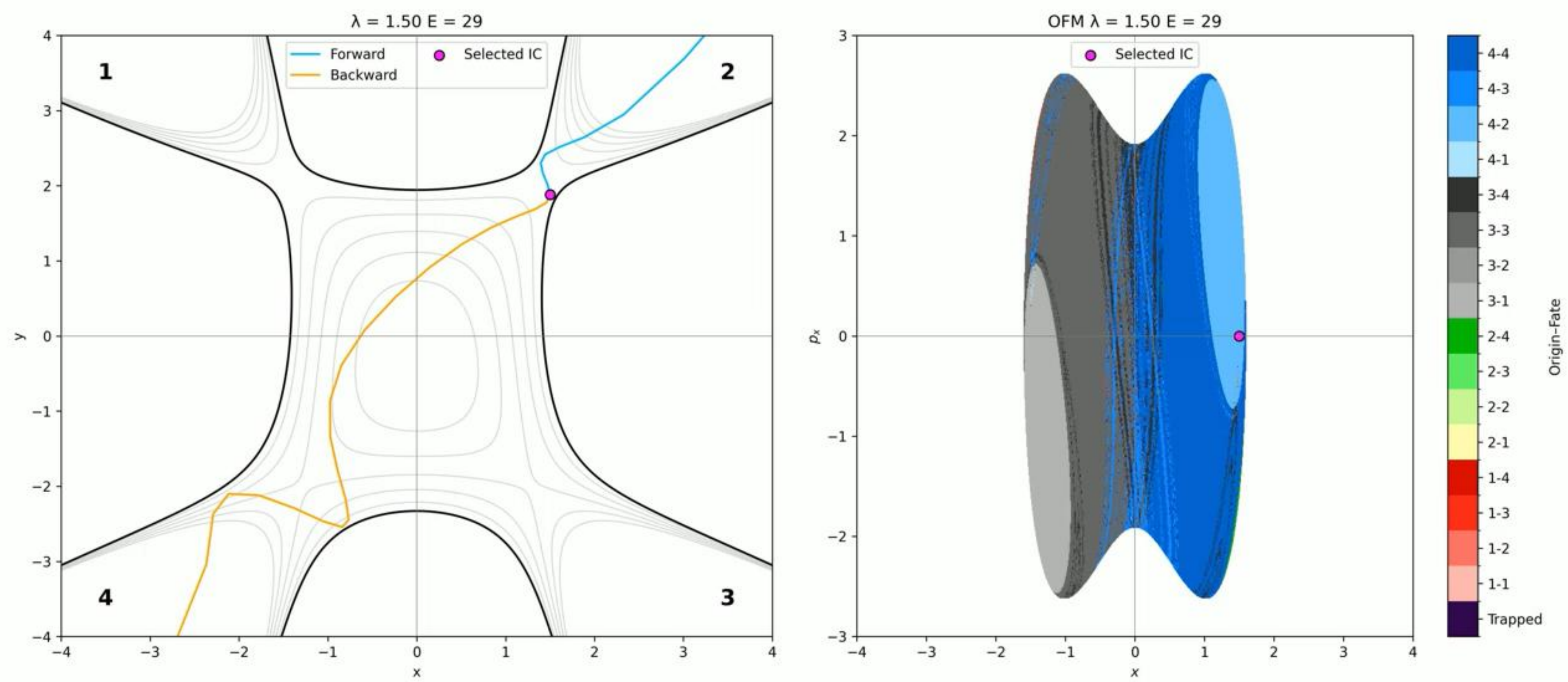


The origin fate map (OFM)

Variation of the stretching parameter $1.5 \geq \lambda \geq 0.6$

PSS: $y = 1.88409,\ p_y > 0, E = 29$. Selected initial condition: $x = 1.5$.

Integration time: $\tau = 20$ time units.

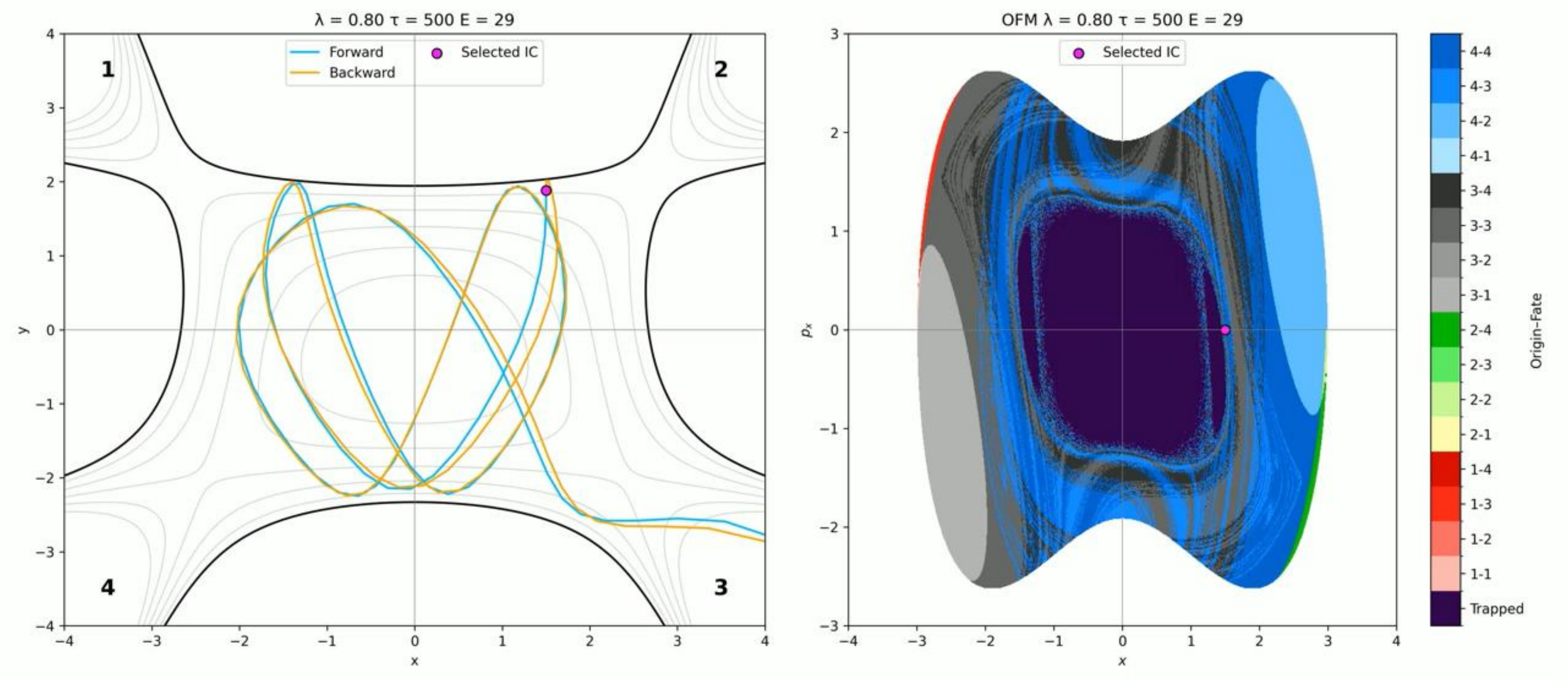


The origin fate map (OFM)

Variation of the stretching parameter $0.8 \geq \lambda \geq 0.6$

PSS: $y = 1.88409,\ p_y > 0, E = 29$. Selected initial condition: $x = 1.5$.

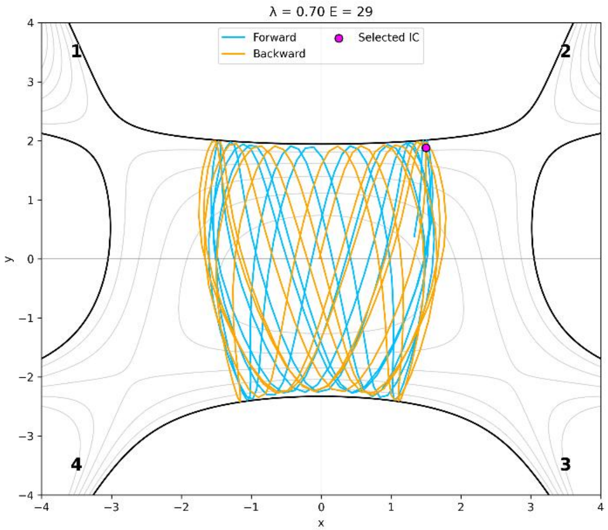
Integration time: $\tau = 500$ time units.

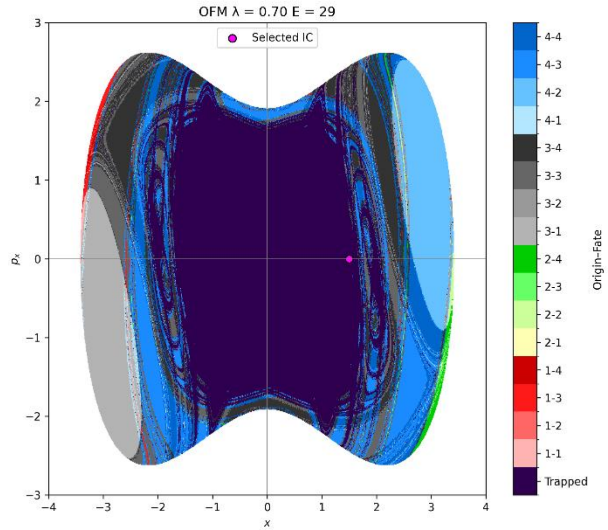


The origin fate map (OFM)

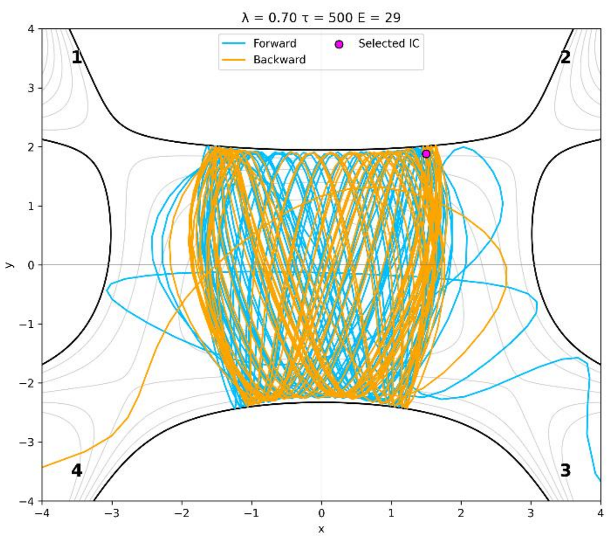
Stretched potential: $\lambda=0.7$

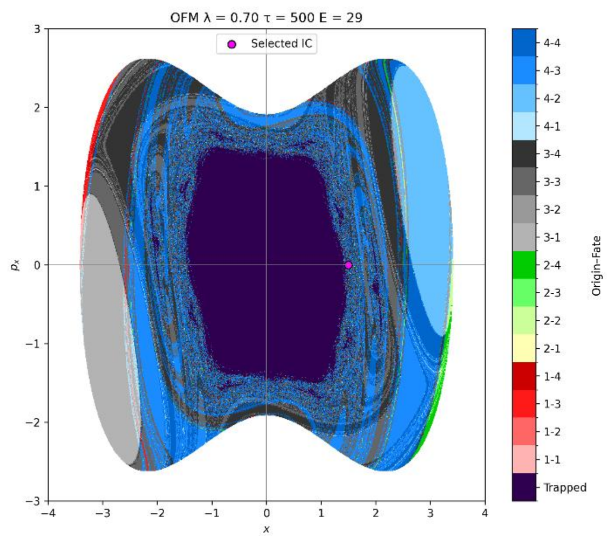
PSS: $y = 1.88409,\ p_y > 0, E = 29$. Selected initial condition: $x = 1.5$.





$\tau = 20$





$\tau = 500$

Lagrangian descriptors (LDs)

The computation of LDs is based on the accumulation of some positive scalar value along the path of individual orbits.

Consider an *N* dimensional continuous time dynamical system

$$\dot{\boldsymbol{x}} = \frac{d\boldsymbol{x}(\boldsymbol{t})}{d\boldsymbol{t}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{t})$$

The arclength definition (Madrid, Mancho, Chaos, 2009 – Mendoza, Mancho, PRL, 2010 – Mancho et al., Commun. Nonlin. Sci. Num. Simul., 2013).

Forward time *LD*:

$$\boldsymbol{LD^f}(\boldsymbol{x}, \boldsymbol{\tau}) = \int_{0}^{\boldsymbol{\tau}} \|\dot{\boldsymbol{x}}(\boldsymbol{t})\| \boldsymbol{dt}$$

Backward time *LD*:

$$\boldsymbol{LD^b}(\boldsymbol{x}, \boldsymbol{\tau}) = \int_{-\boldsymbol{\tau}}^{0} \|\dot{\boldsymbol{x}}(\boldsymbol{t})\| \boldsymbol{dt}$$

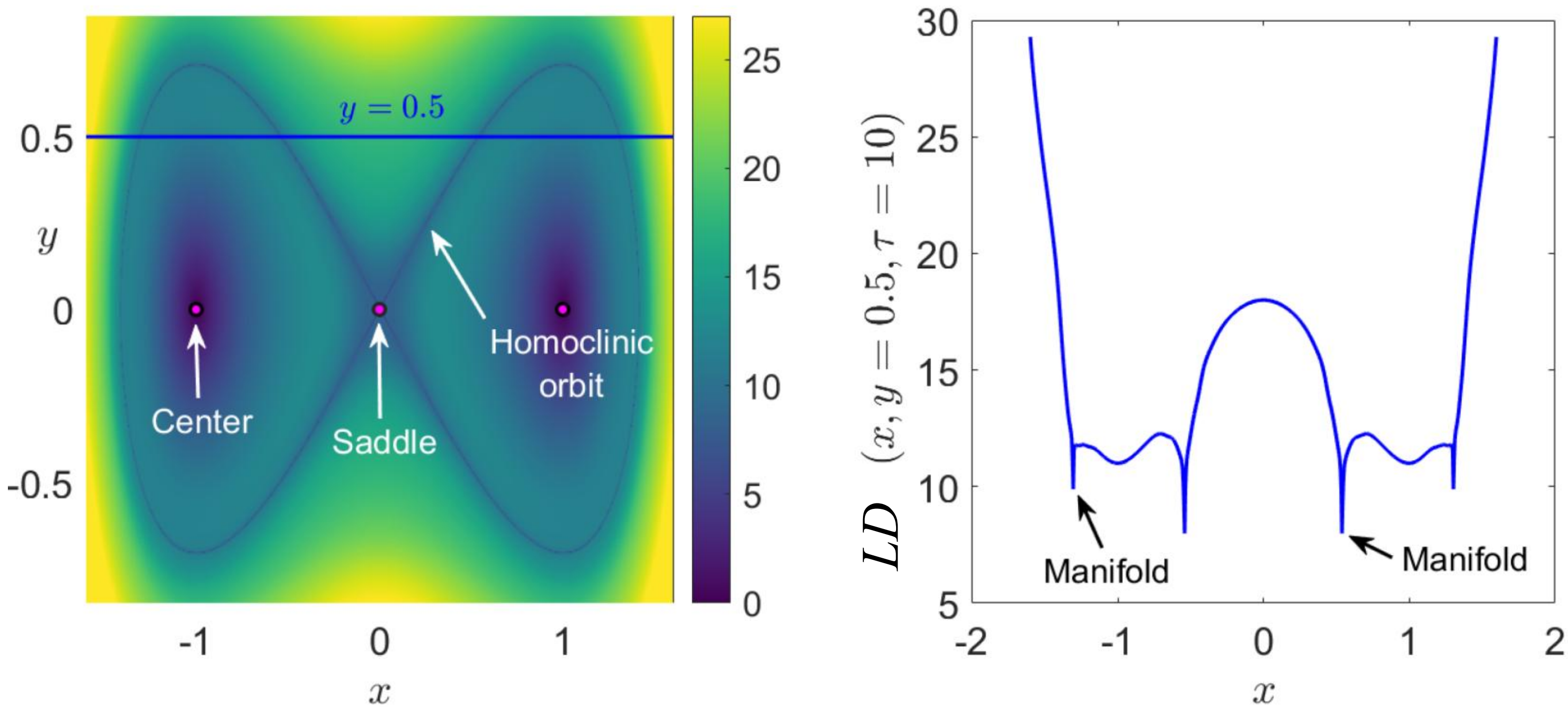
Combined *LD*:

$$\boldsymbol{LD}(\boldsymbol{x}, \boldsymbol{\tau}) = \boldsymbol{LD^b}(\boldsymbol{x}, \boldsymbol{\tau}) + \boldsymbol{LD^f}(\boldsymbol{x}, \boldsymbol{\tau})$$

LDs: 1 dof Duffing Oscillator

$$H(x,y) = \frac{1}{2}y^2 + \frac{1}{4}x^4 - \frac{1}{2}x^2$$

The system has three equilibrium points: a saddle located at the origin and two diametrically opposed centers at the points (± 1, 0).



From Agaoglou et al. 'Lagrangian descriptors: Discovery and quantification of phase space structure and transport', 2020, https://doi.org/10.5281/zenodo.3958985

The location of the stable and unstable manifolds can be extracted from the ridges of the gradient field of the LDs since they are located at points where the forward and the backward components of the LD are non-differentiable.

Lagrangian descriptors (LDs)

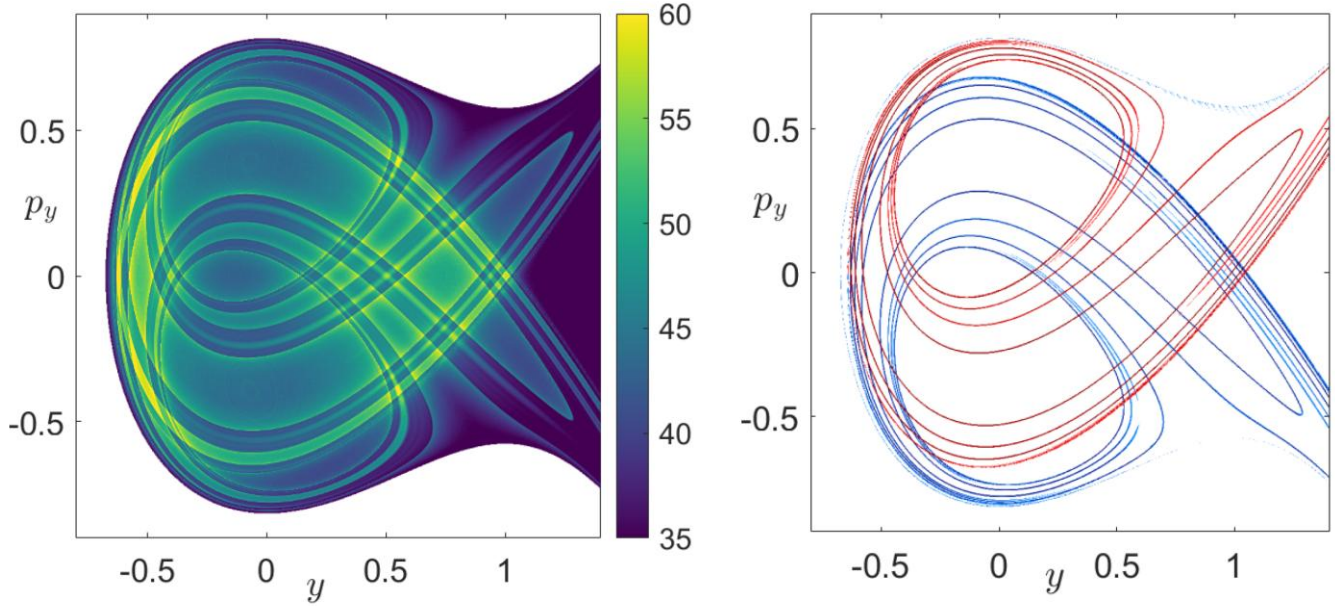
The '*p*-norm' definition (Lopesino et al., Commun. Nonlin. Sci. Num. Simul., 2015 – Lopesino et al., Int. J. Bifurcat. Chaos, 2017).

Combined *LD* (usually *p*=1/2):

$$\boldsymbol{LD}(\boldsymbol{x},\boldsymbol{\tau}) = \int_{-\tau}^{\tau}\left(\sum_{i=1}^{N}|f_i(\boldsymbol{x},t)|^p\right)dt$$

Hénon-Heiles system: $H = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3$

Stable and unstable manifolds for H=1/3, τ=10.



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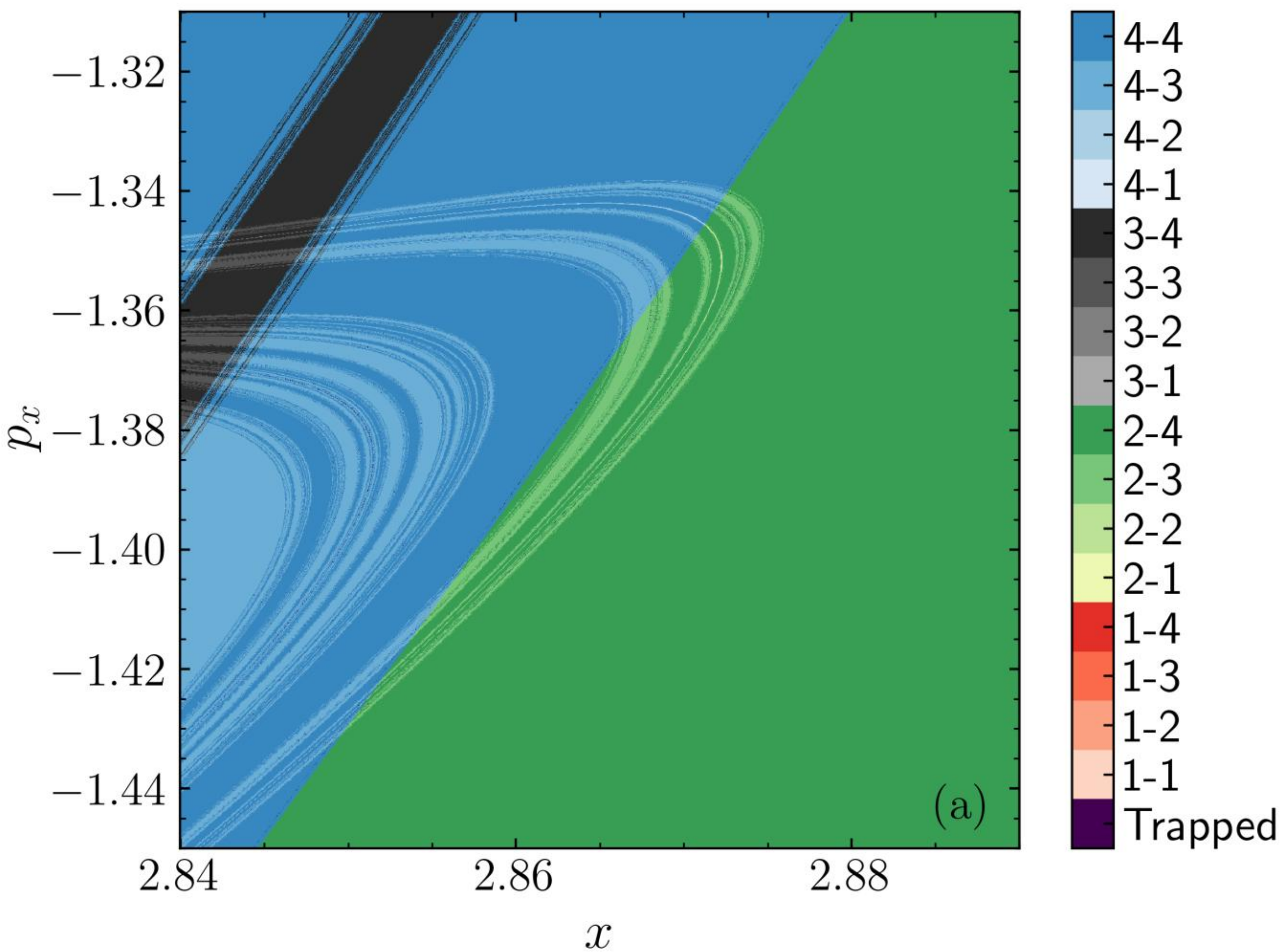
OFM and manifold dynamics

Stretched potential: λ=0.778

PSS: $y = 1.88409,\ p_y > 0, E = 29$. Integration time: $\tau = 20$ time units.



OFM and manifold dynamics

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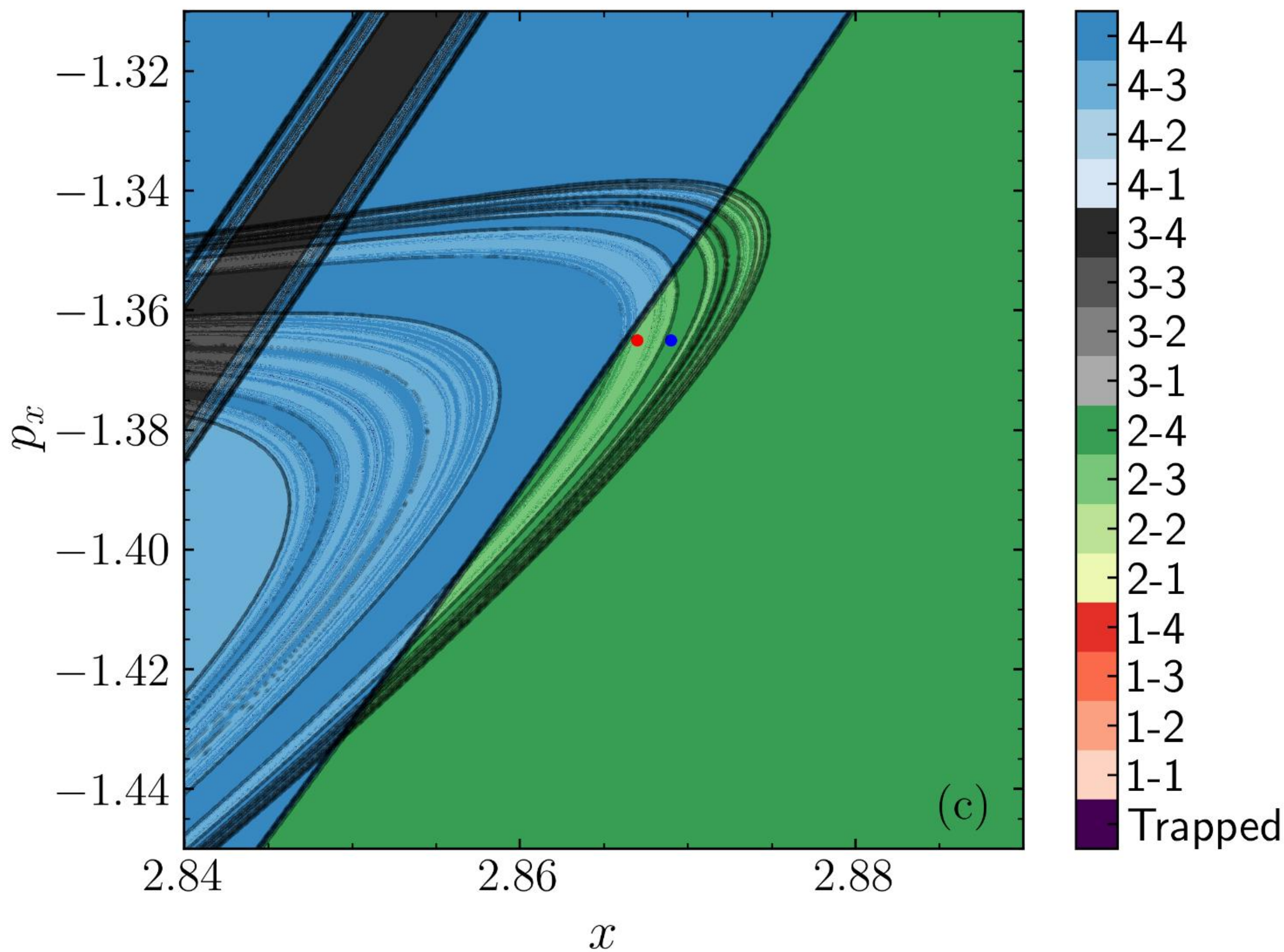

OFM and manifold dynamics

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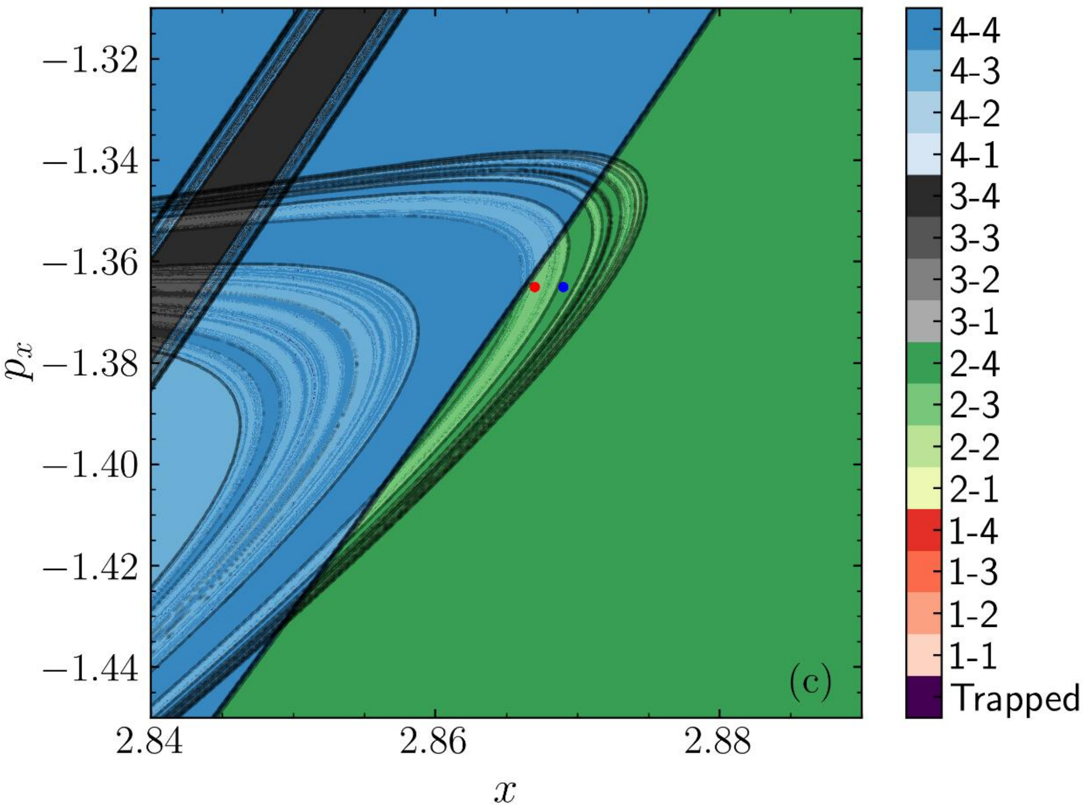
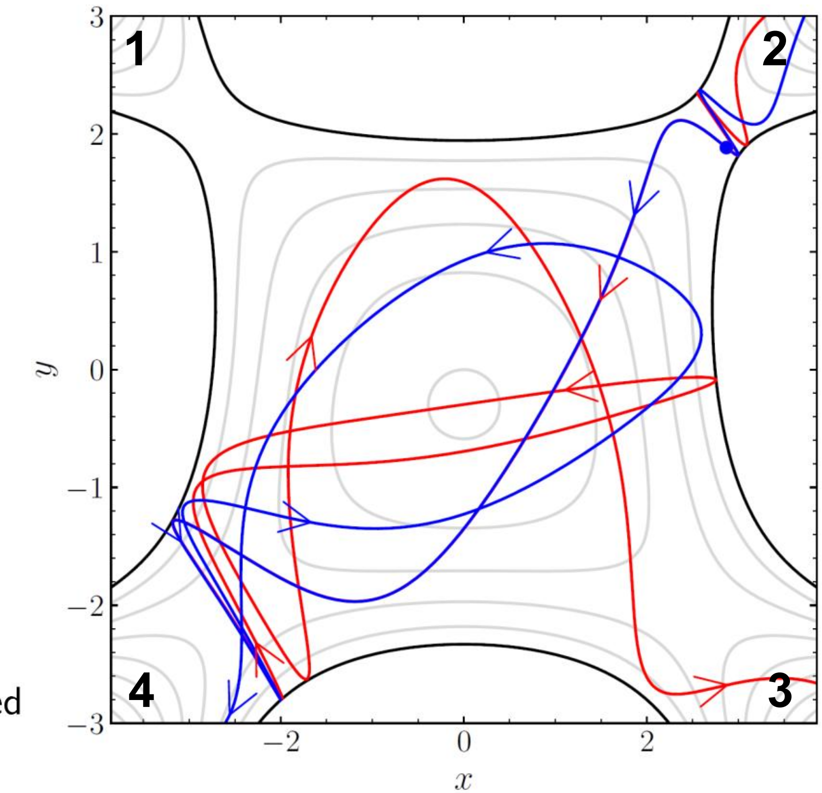




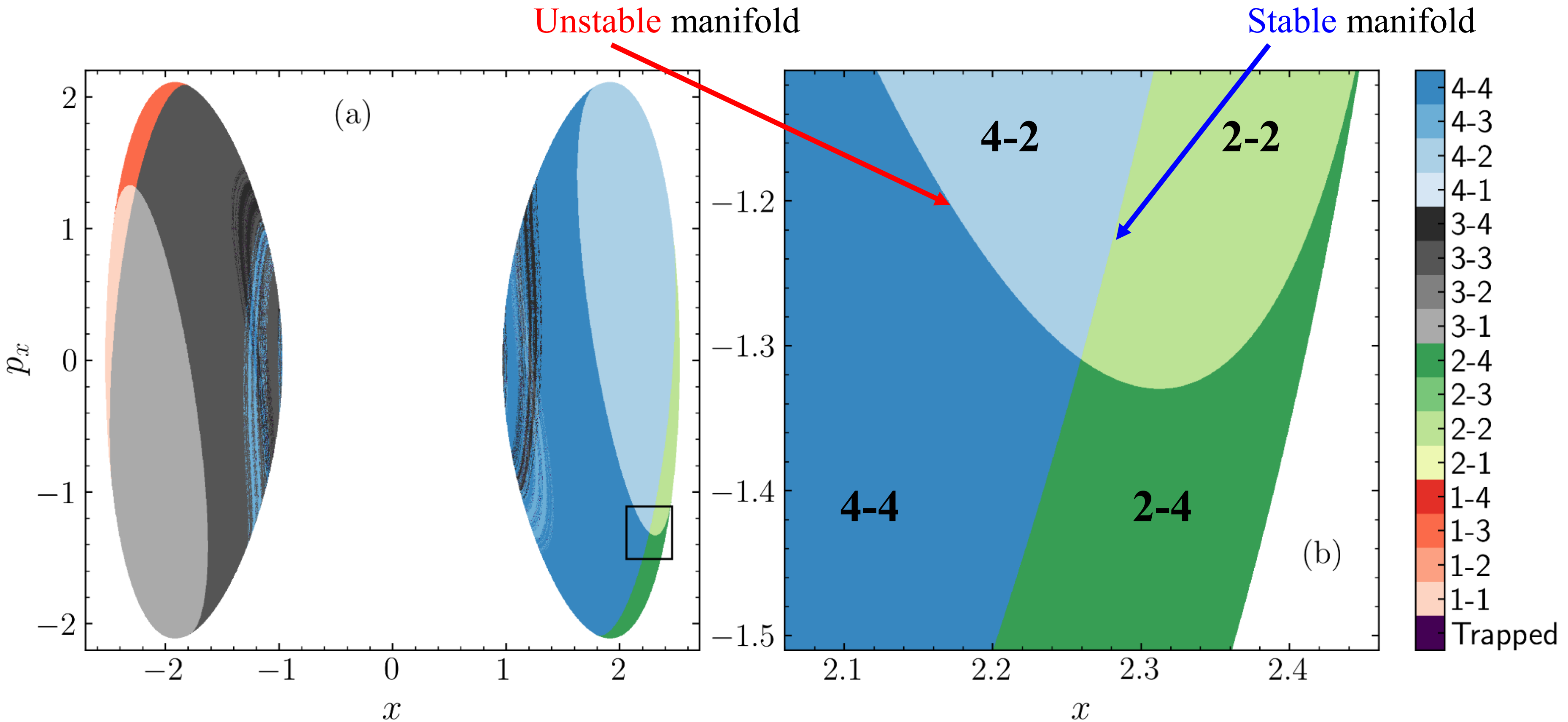
$$\left(x, y, p_x, p_y\right) = (2.876, 1.88409, -1.365, 0.86563646)$$

$$\left(x, y, p_x, p_y\right) = (2.869, 1.88409, -1.365, 0.85272480)$$

Locating unstable periodic orbits (UPOs)

UPOs are located at the intersection of stable and unstable manifolds, i.e. at corner points of the OFM.

Change in the origin (fate) index: crossing of a stable (unstable) manifold, which governs backward (forward)-time transport.



Symmetric potential: λ=1.0. PSS: $y = 2.0,\ p_y > 0, E = 29, \tau = 20.$

Summary

- Origin fate map: coloring initial conditions according to both their past (origin – backward time integration) and their future (fate – forward time integration) evolution.
- Clear visualization of the system's dynamics and phase space transport along with their evolution in time.
- Revelation of both stable and unstable manifold behavior.
- Assist the accurate estimation of the position of unstable periodic orbits.
- The idea of the OFT is straightforwardly extensible to different open Hamiltonian models with escapes, and to dissipative systems with forward- and backward-time attractors.
- The technique works for Hamiltonian and non-Hamiltonian systems.
- The definition of an origin/fate state depends on the properties of the system, and could be an attractor, escape channel, spatially localized region, etc.

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