

Numerical methods for studying the behavior of low-dimensional nonlinear dynamical systems

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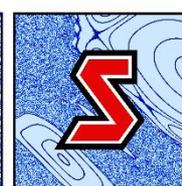
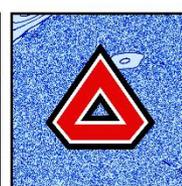
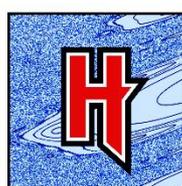
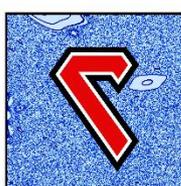
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MAX-PLANCK-INSTITUT
FÜR PHYSIK KOMPLEXER SYSTEME

Outline

- Lagrangian descriptors (LDs)
- Smaller Alignment Index (SALI)
- Chaos diagnostics based on LDs:
 - ✓ the difference of LDs of neighboring orbits
 - ✓ the ratio of LDs of neighboring orbits
 - ✓ a quantity related to the finite-difference second spatial derivative of LDs
 - ✓ Applications: Hénon – Heiles system, 2D Standard map, 4D Standard map
- The origin fate map (OFM)
 - ✓ The 2 degree of freedom caldera Hamiltonian system
 - ✓ Definition of the OFM
 - ✓ Visualization of phase space transport
 - ✓ Relation to the morphology of manifolds
 - ✓ Locating the position of unstable periodic orbits
- Summary

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

$$\dot{x} = \frac{dx(t)}{dt} = f(x, t)$$

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

Forward time LD :

$$LD^f(x, \tau) = \int_0^\tau \|\dot{x}(t)\| dt$$

Backward time LD :

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

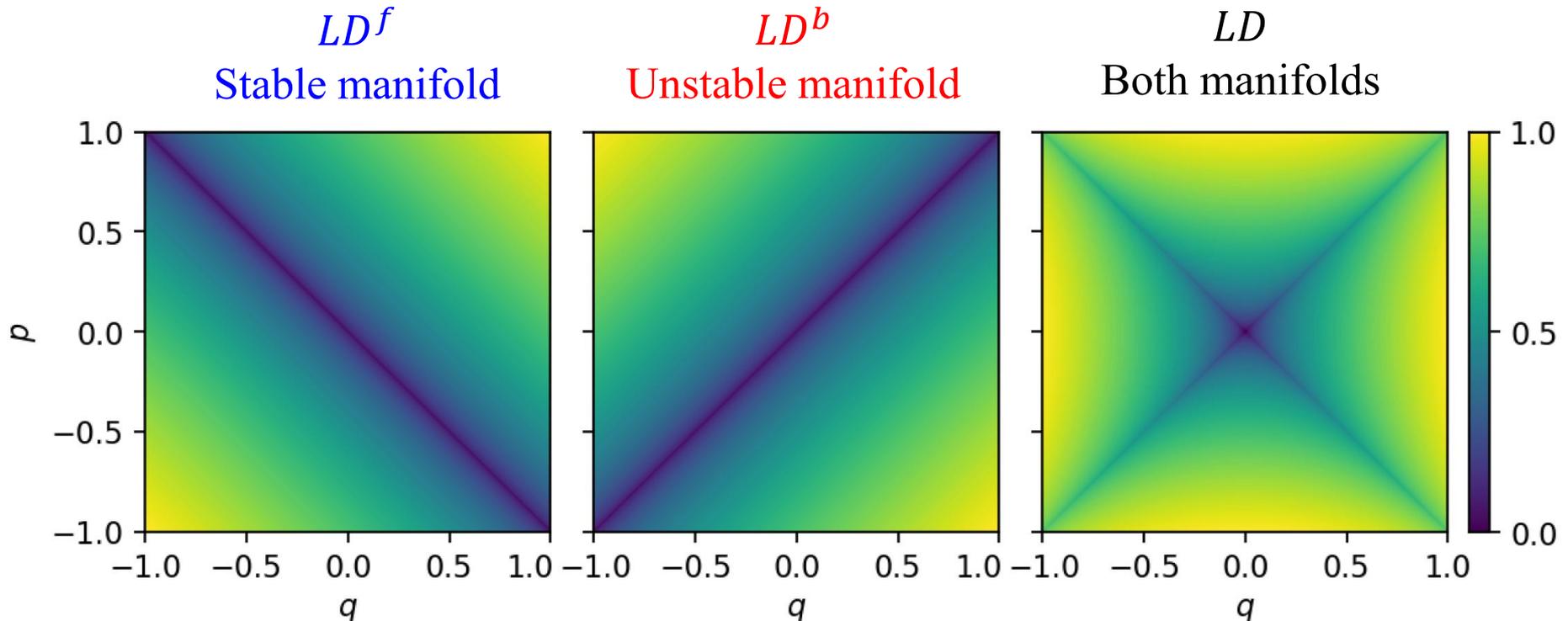
Combined LD :

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

LDs: 1 degree of freedom (dof) Hamiltonian

$$H(q, p) = \frac{1}{2} (p^2 - q^2)$$

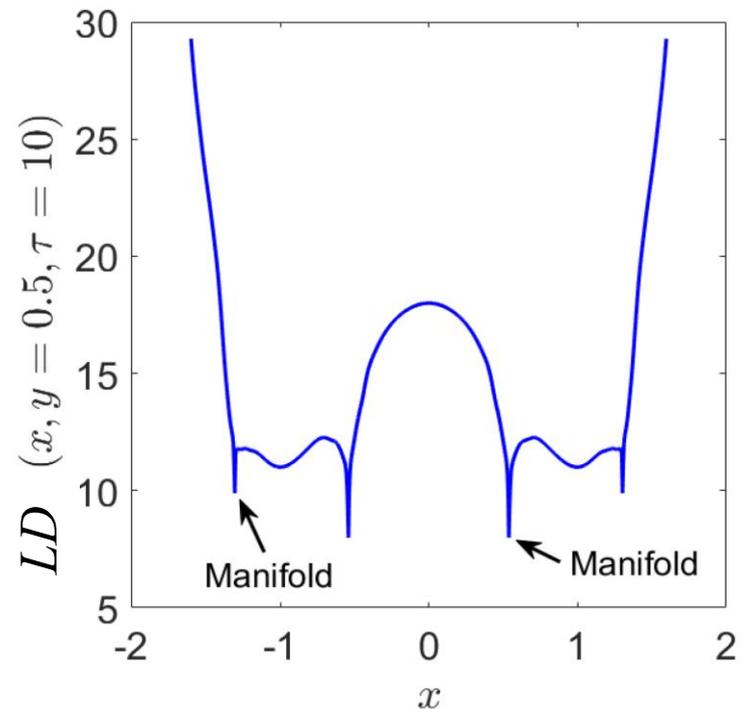
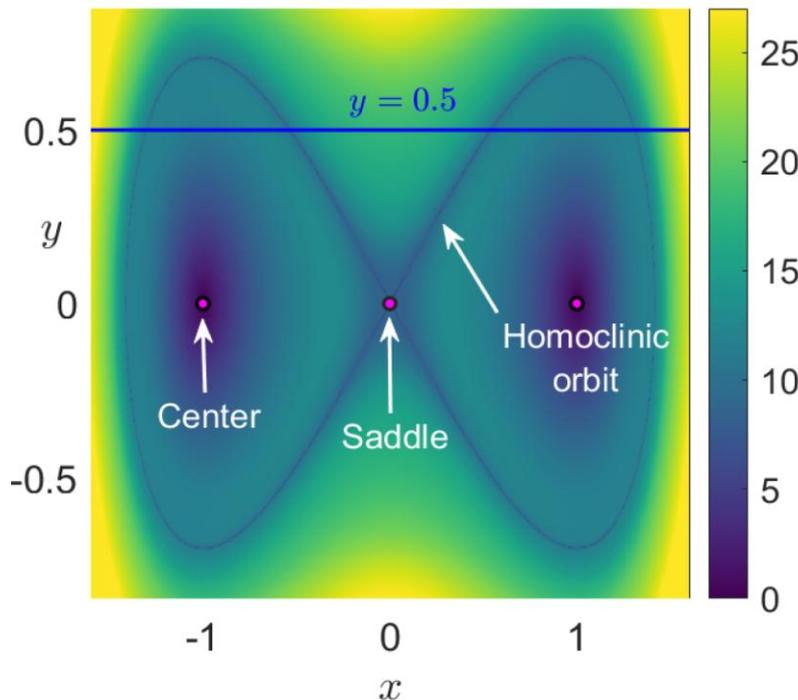
The system has a hyperbolic fixed point at the origin. The LDs can be used to display the stable and unstable manifolds of this point.



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 $(\pm 1, 0)$.



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)

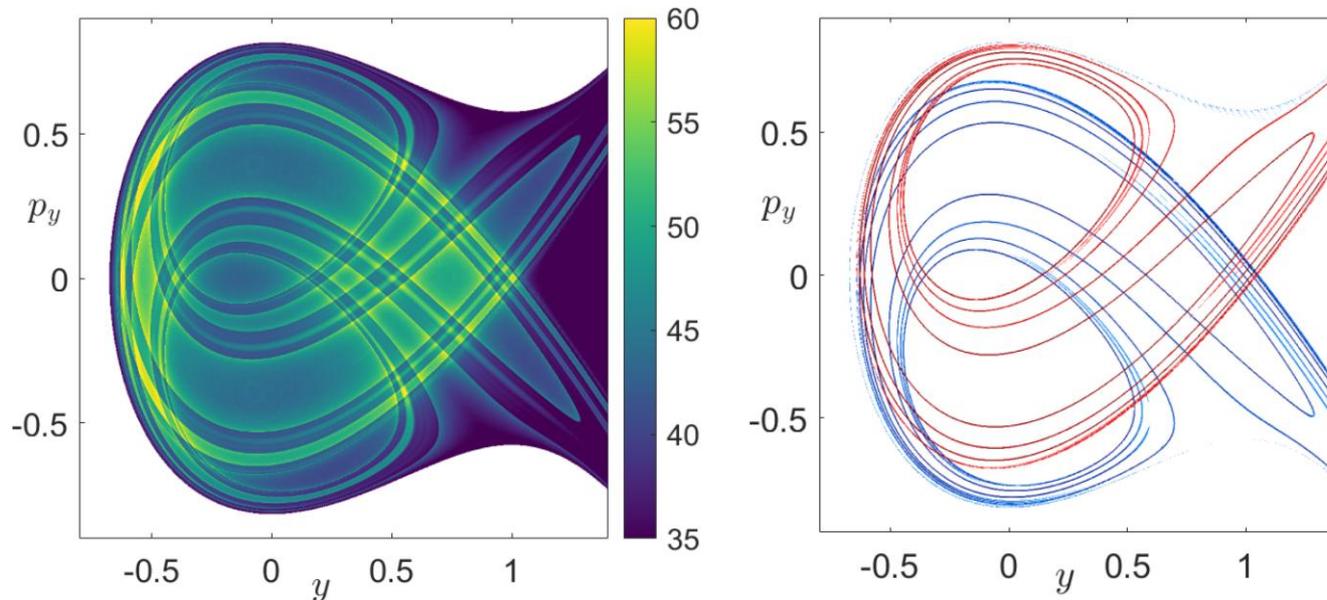
The '*p*-norm' definition (Lopesino et al., Commun. Nonlin. Sci. Num. Simul., 2015 – Lopesino et al., Int. J. Bifurcat. Chaos, 2017).

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

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

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 $H=1/3$, $\tau=10$.



Maximum Lyapunov Exponent (MLE)

Chaos: sensitive dependence on initial conditions.

Roughly speaking, the MLE of a given orbit characterizes the **mean exponential rate of divergence** of trajectories surrounding it.

Consider an orbit in the $2N$ -dimensional phase space with **initial condition $x(0)$** and **an initial deviation vector (small perturbation) from it $v(0)$** .

Then the mean exponential rate of divergence is:

$$MLE = \lambda_1 = \lim_{t \rightarrow \infty} \Lambda(t) = \lim_{t \rightarrow \infty} \frac{1}{t} \ln \frac{\|v(t)\|}{\|v(0)\|}$$

$\lambda_1 = 0 \rightarrow$ Regular motion ($\Lambda \propto t^{-1}$)

$\lambda_1 > 0 \rightarrow$ Chaotic motion

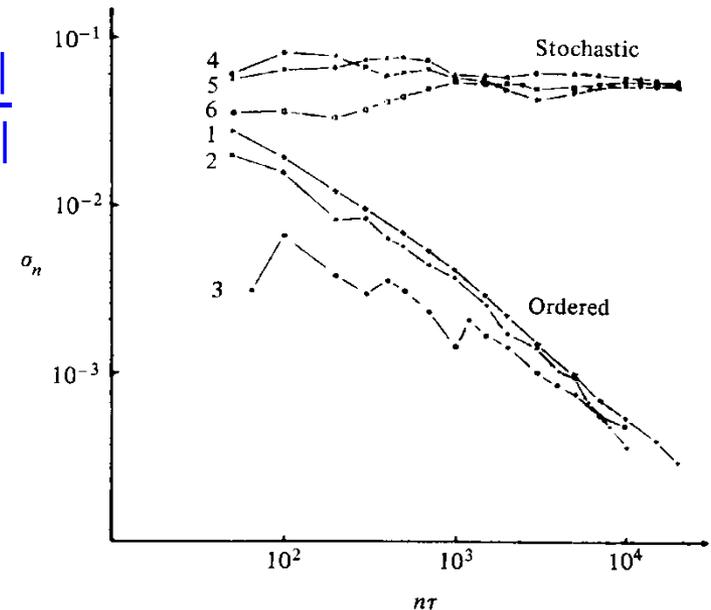


Figure 5.7. Behavior of σ_n at the intermediate energy $E = 0.125$ for initial points taken in the ordered (curves 1–3) or stochastic (curves 4–6) regions (after Benettin *et al.*, 1976).

The Smaller Alignment Index (SALI)

Consider the $2N$ -dimensional phase space of a conservative dynamical system (symplectic map or Hamiltonian flow).

An orbit in that space with initial condition :

$$P(0) = (x_1(0), x_2(0), \dots, x_{2N}(0))$$

and a deviation vector

$$v(0) = (\delta x_1(0), \delta x_2(0), \dots, \delta x_{2N}(0))$$

The evolution in time (in maps the time is discrete and is equal to the number n of the iterations) of a deviation vector is defined by:

- the variational equations (for Hamiltonian flows) and
- the equations of the tangent map (for mappings)

Definition of the SALI

We follow the evolution in time of two different initial deviation vectors ($v_1(0)$, $v_2(0)$), and define SALI [S., J. Phys. A (2001) – S. & Manos, Lect. Notes Phys. (2016)] as:

$$SALI(t) = \min\{\|\hat{v}_1(t) + \hat{v}_2(t)\|, \|\hat{v}_1(t) - \hat{v}_2(t)\|\}$$

where

$$\hat{v}_1(t) = \frac{v_1(t)}{\|v_1(t)\|}$$

When the two vectors become collinear

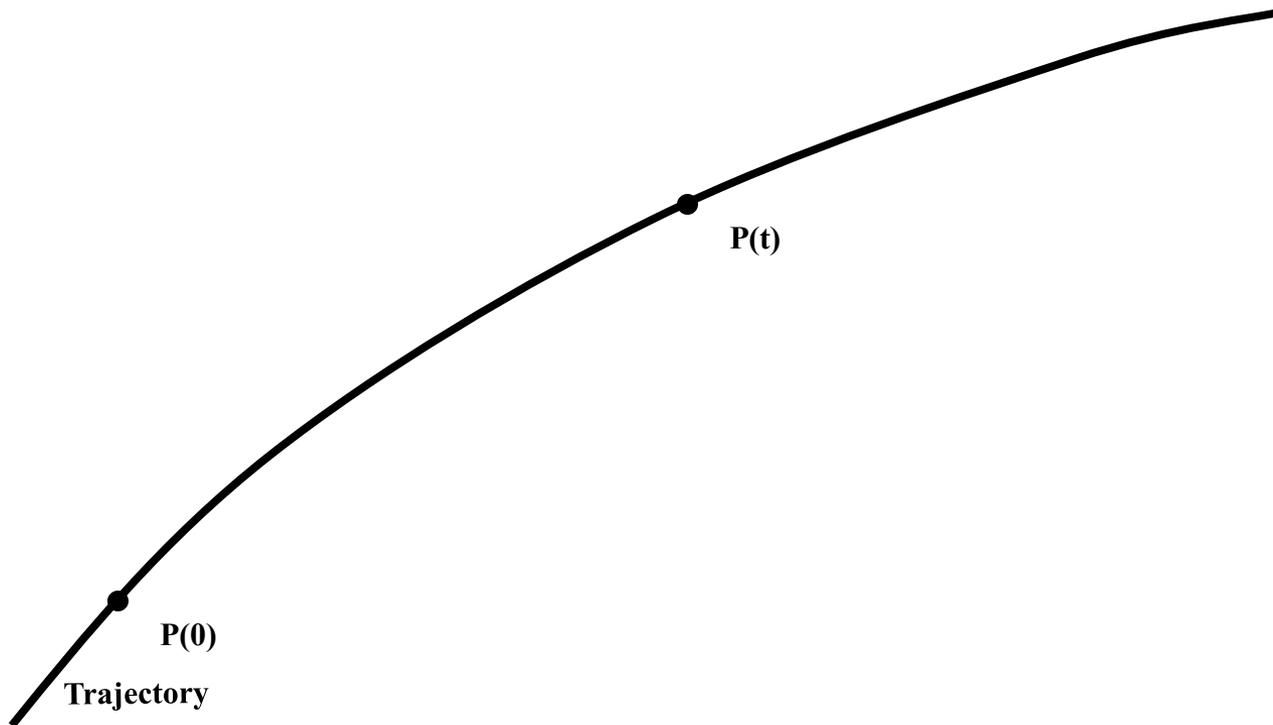
$$SALI(t) \rightarrow 0$$

Behavior of SALI for **chaotic motion**

For chaotic orbits the two initially different deviation vectors tend to coincide with the direction defined by the maximum Lyapunov exponent.

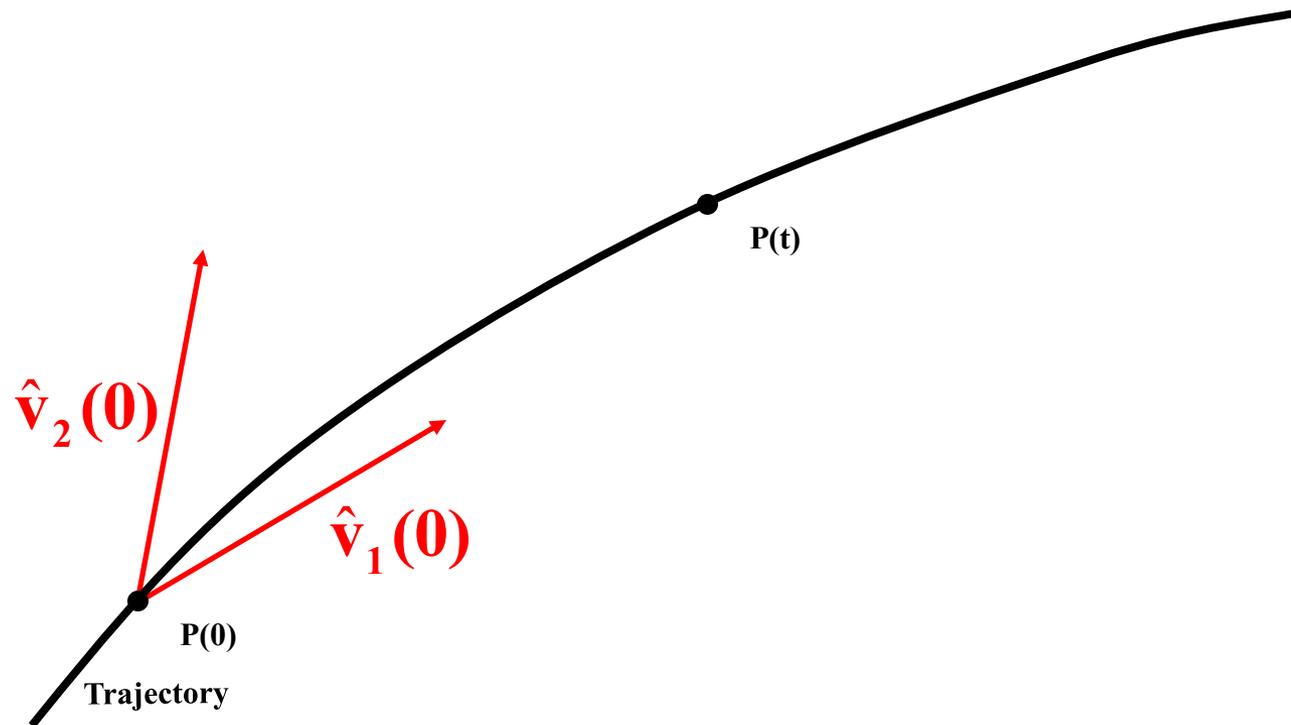
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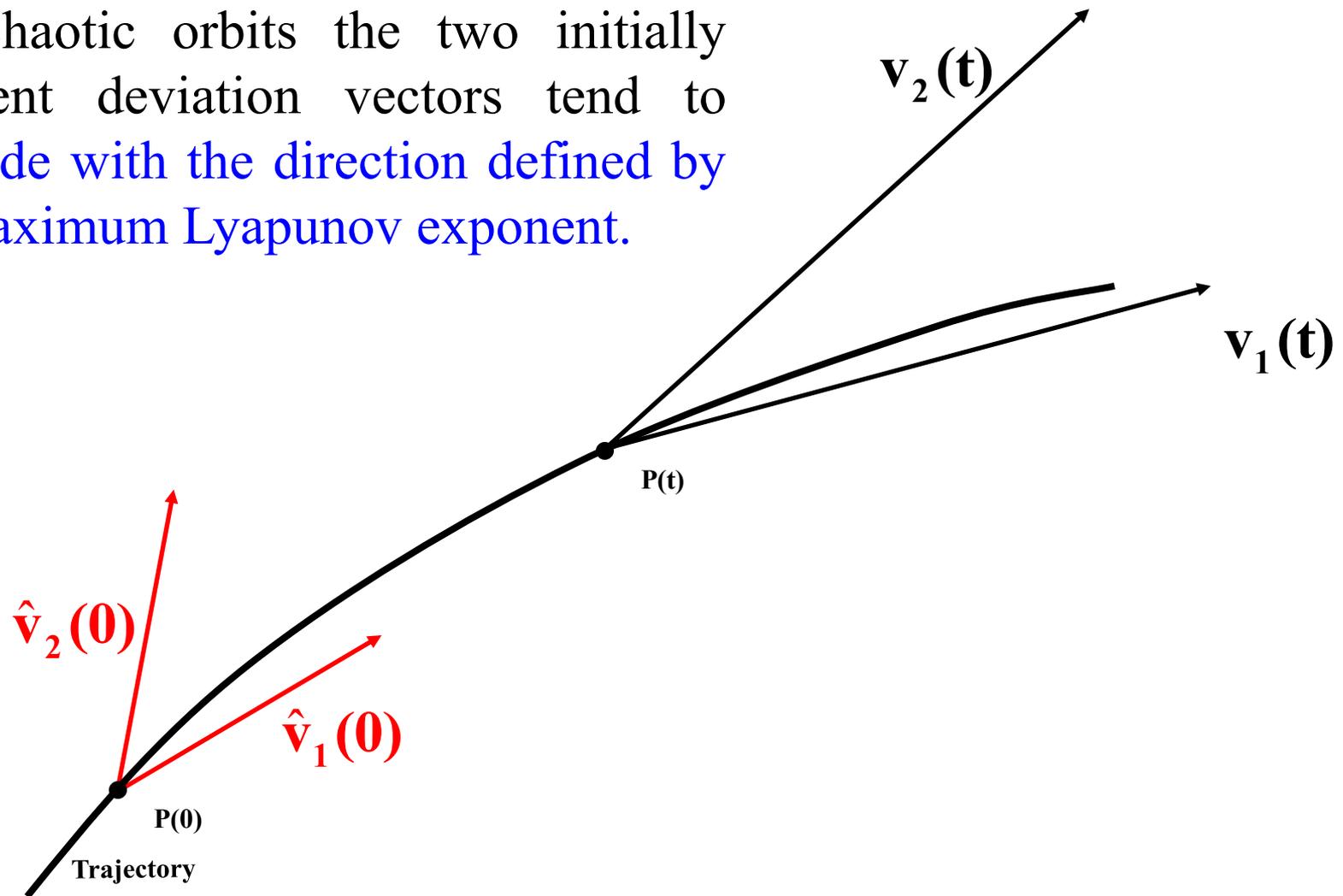
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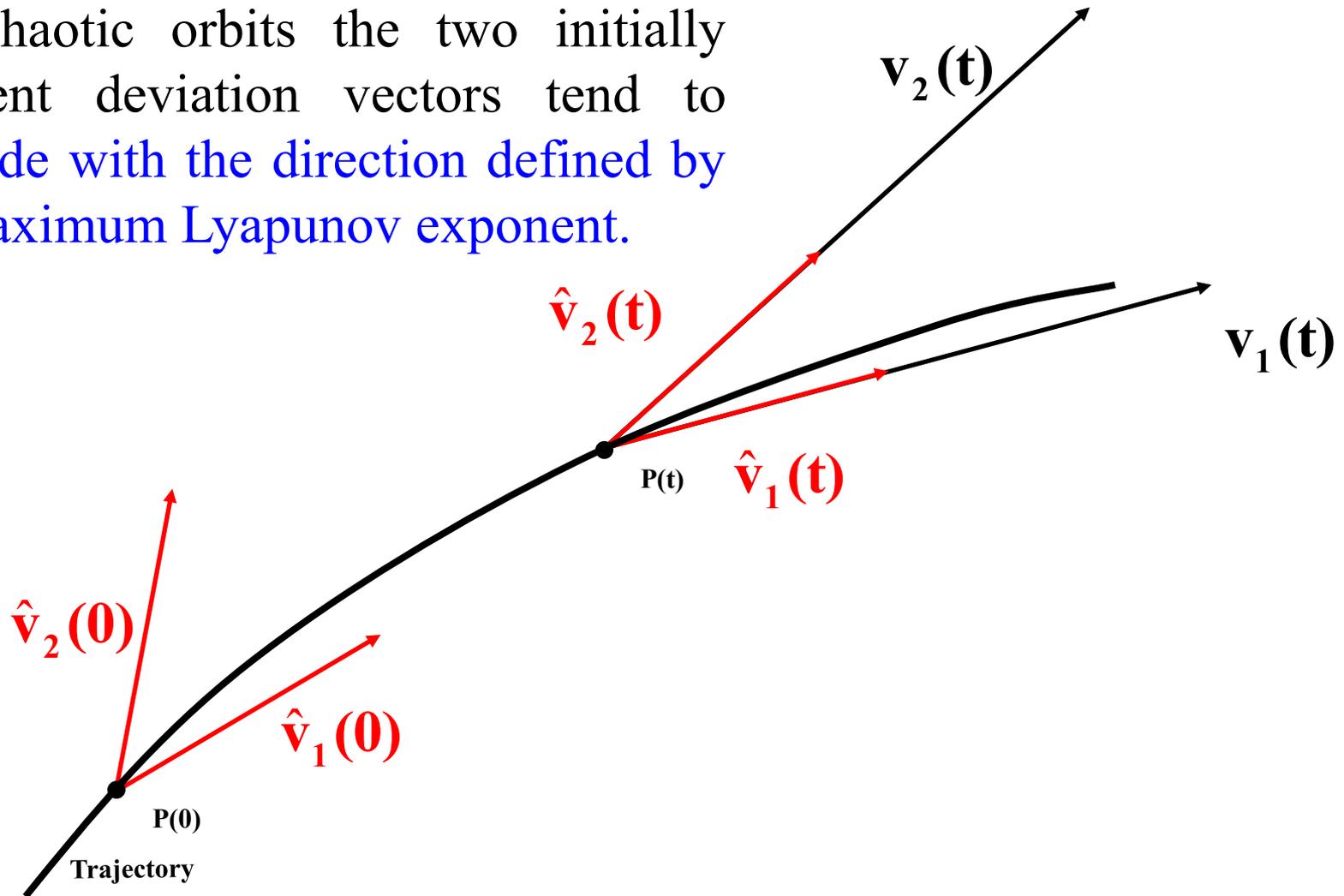
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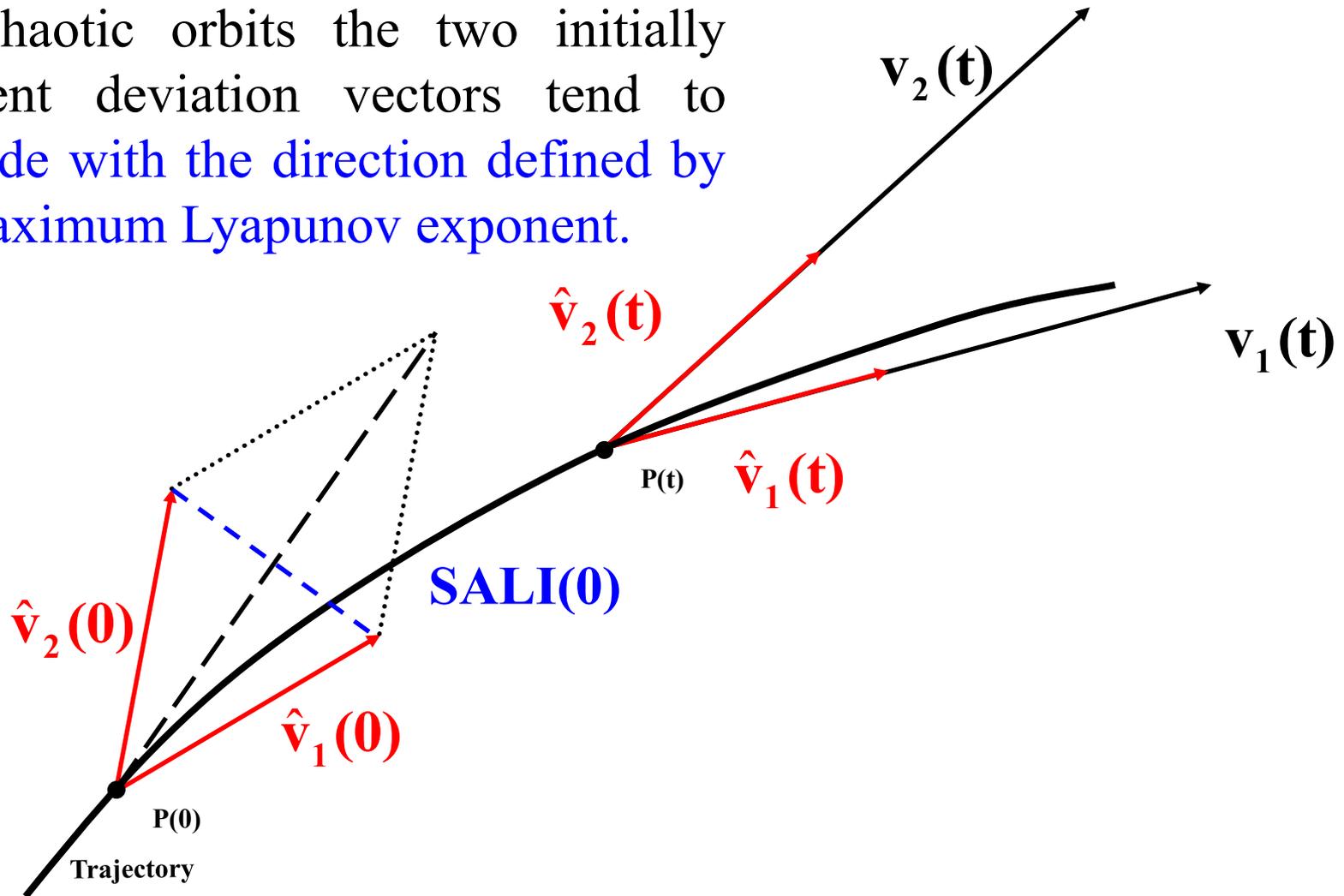
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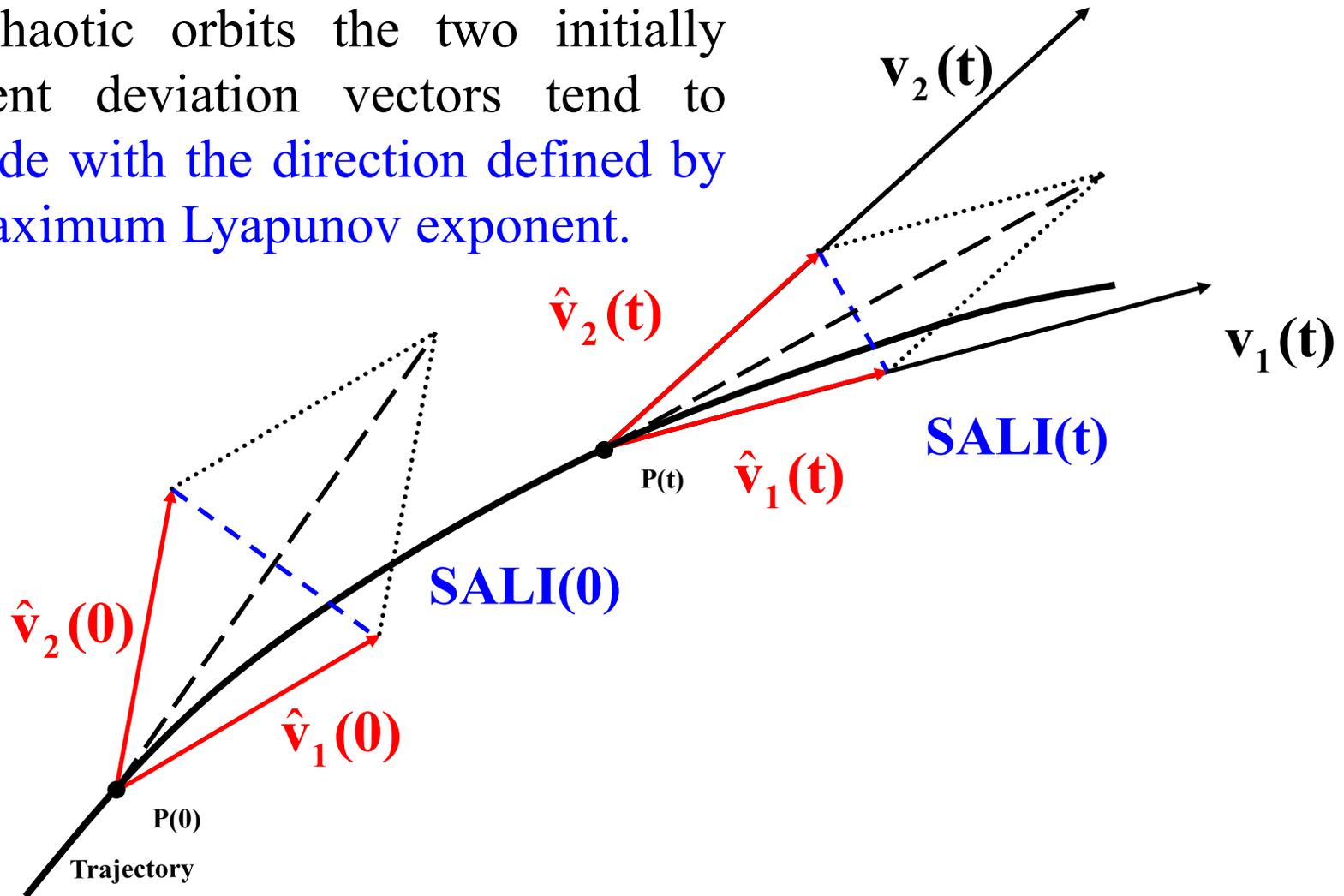
Behavior of SALI for chaotic motion

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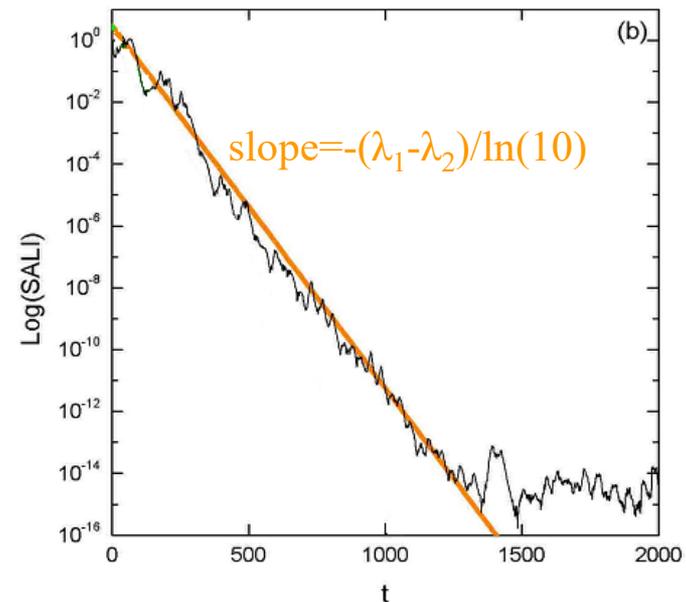
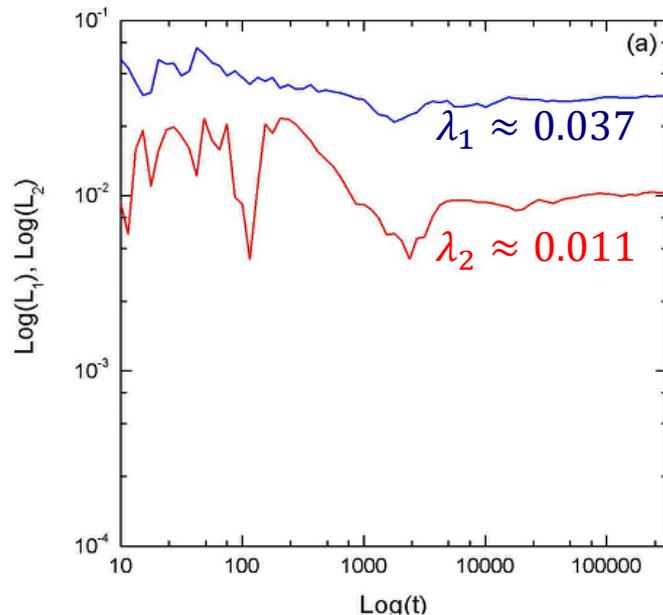


Behavior of the SALI for chaotic motion

We test the validity of the approximation $SALI \propto e^{-(\lambda_1 - \lambda_2)t}$ [S. et al., J. Phys. A (2004)] for a chaotic orbit of the 3D Hamiltonian

$$H = \sum_{i=1}^3 \frac{\omega_i}{2} (q_i^2 + p_i^2) + q_1^2 q_2 + q_1^2 q_3$$

with $\omega_1=1$, $\omega_2=1.4142$, $\omega_3=1.7321$, $H=0.09$

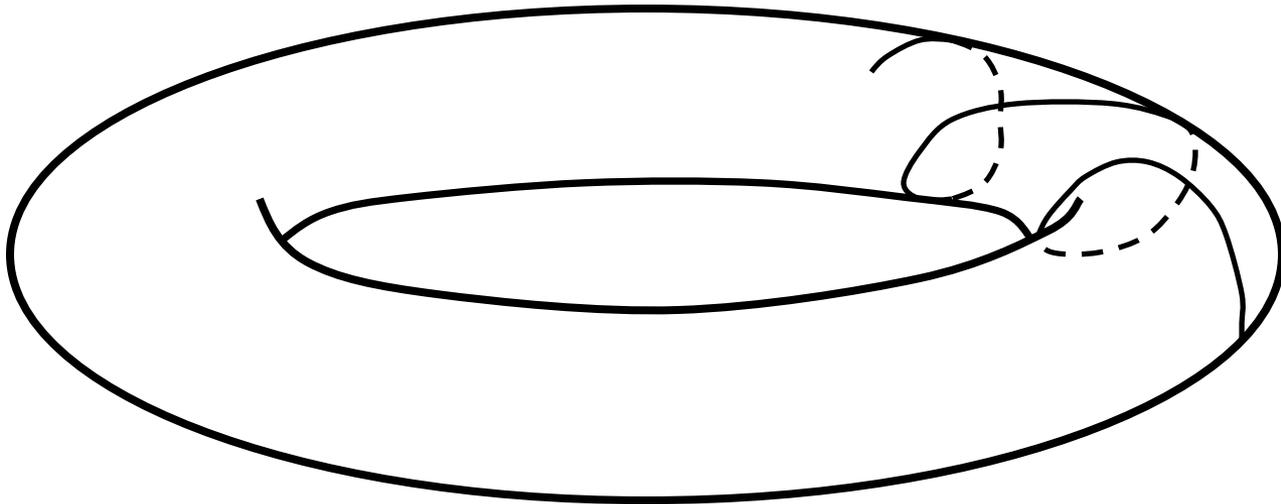


Behavior of SALI for regular motion

Regular motion occurs on a torus and two different initial deviation vectors become tangent to the torus, generally having different directions.

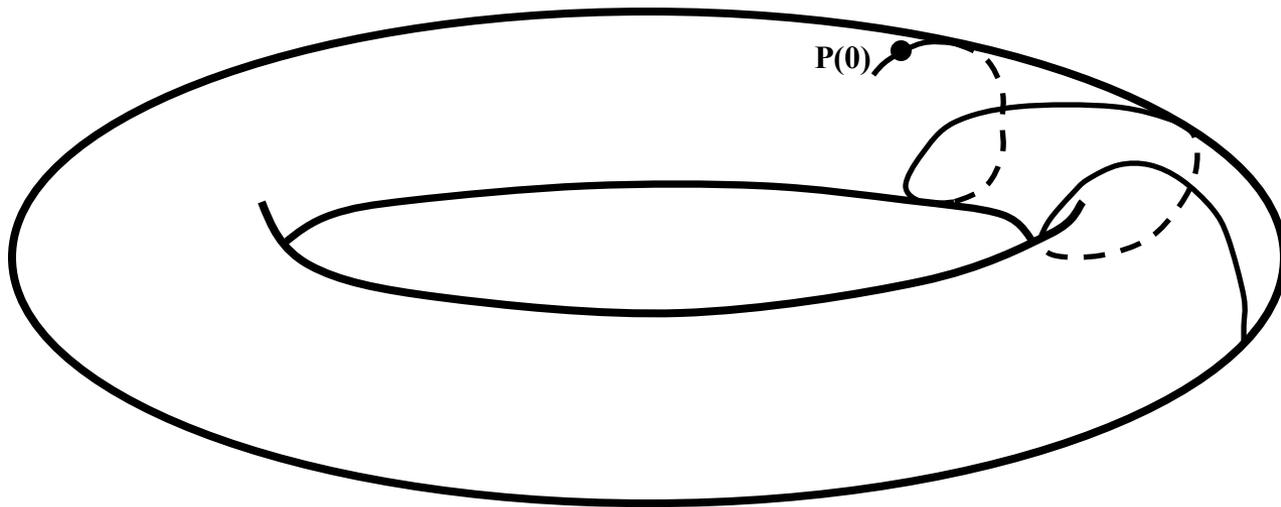
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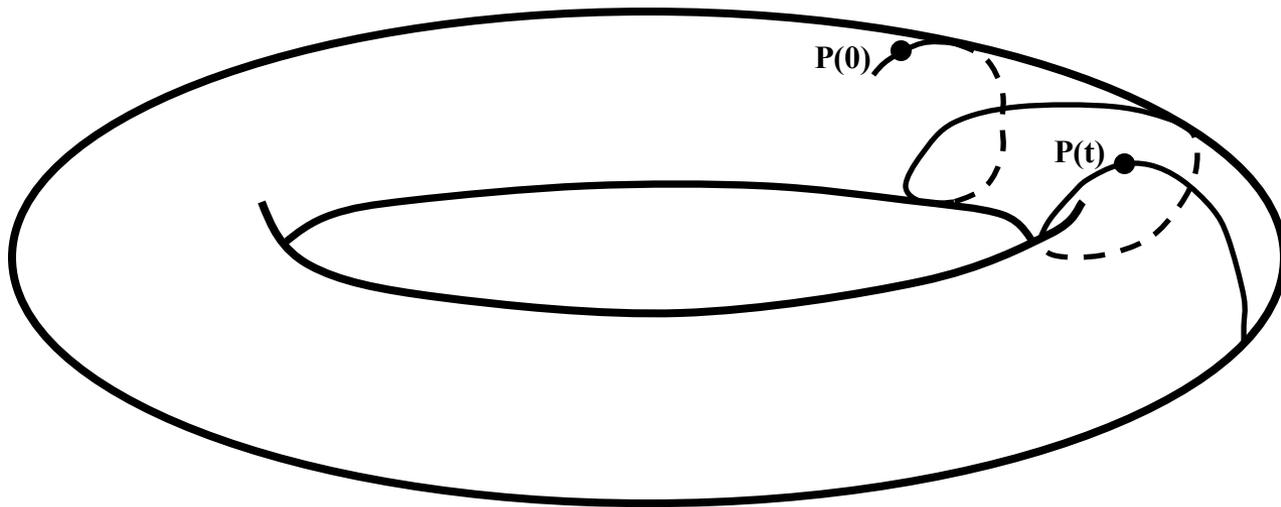
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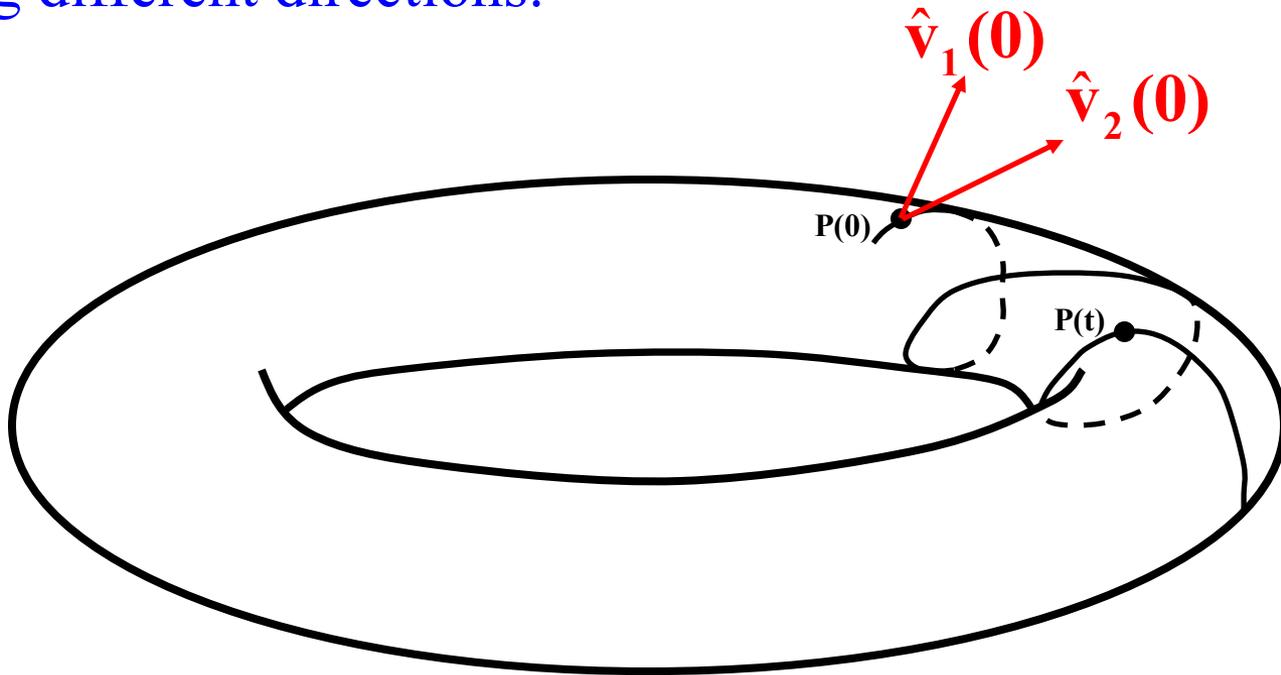
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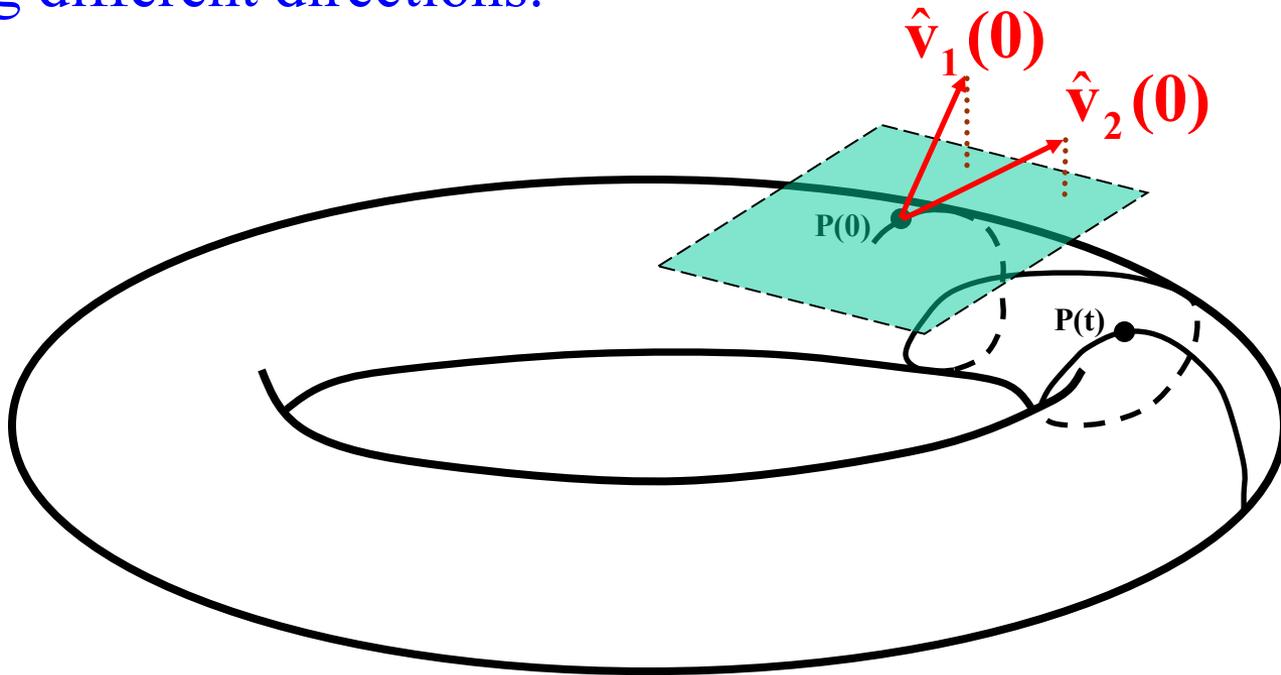
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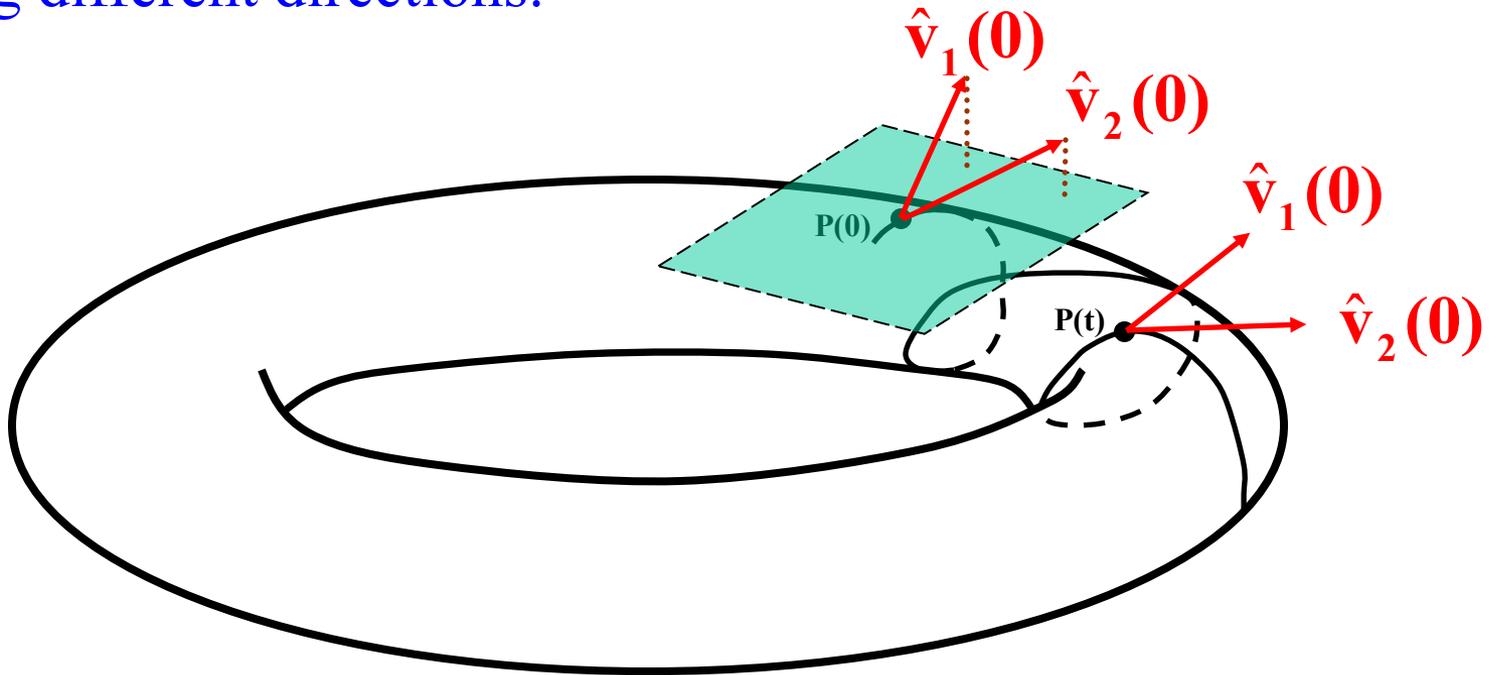
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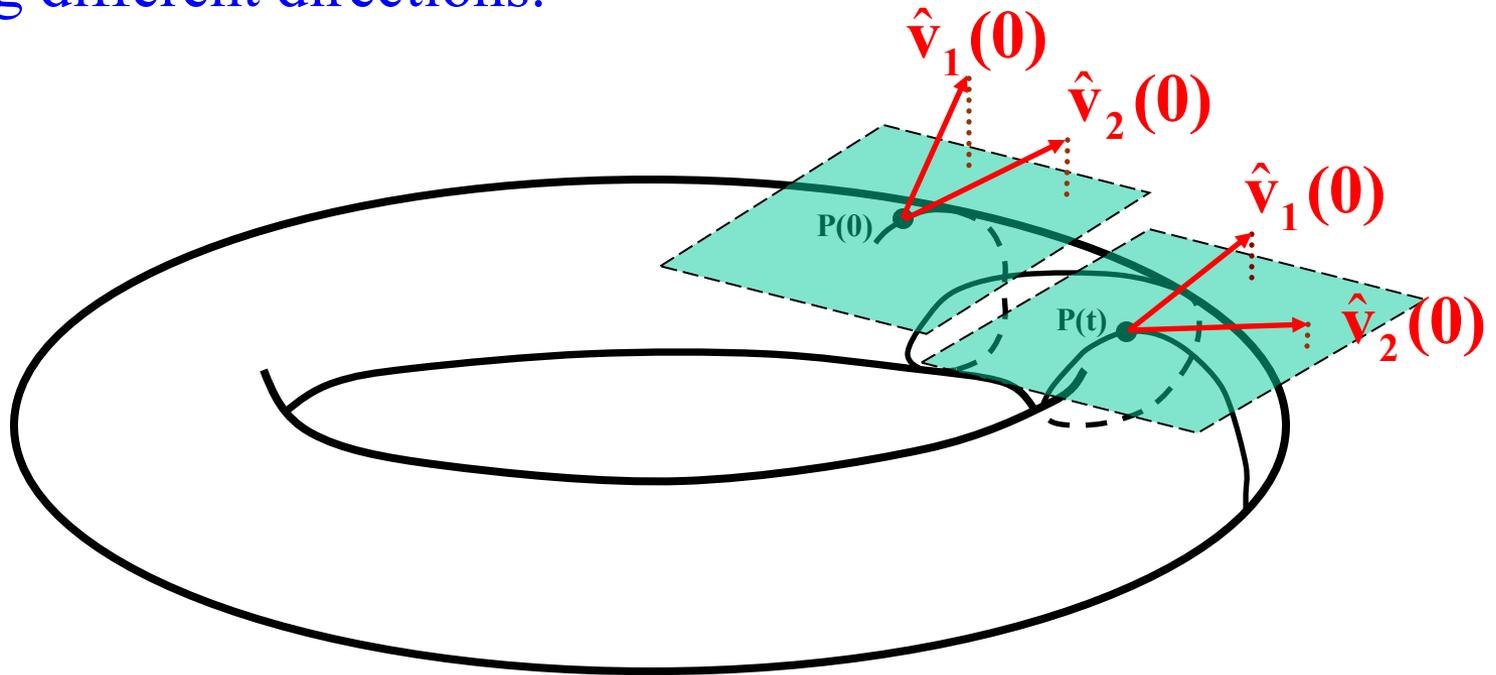
Behavior of SALI for regular motion

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Behavior of SALI for regular motion

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SALI – Hénon-Heiles system

As an example, we consider the 2D Hénon-Heiles system:

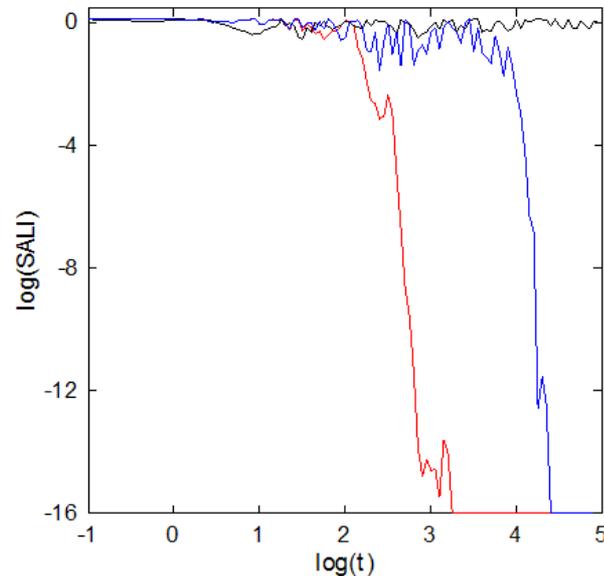
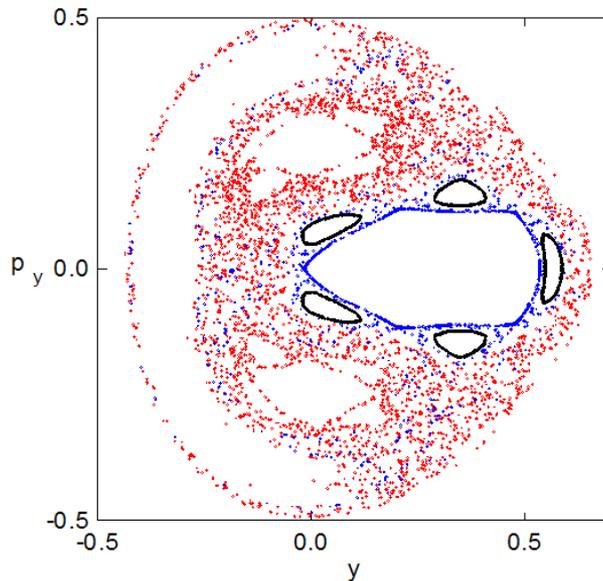
$$H = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3$$

For $E=1/8$ we consider the orbits with initial conditions:

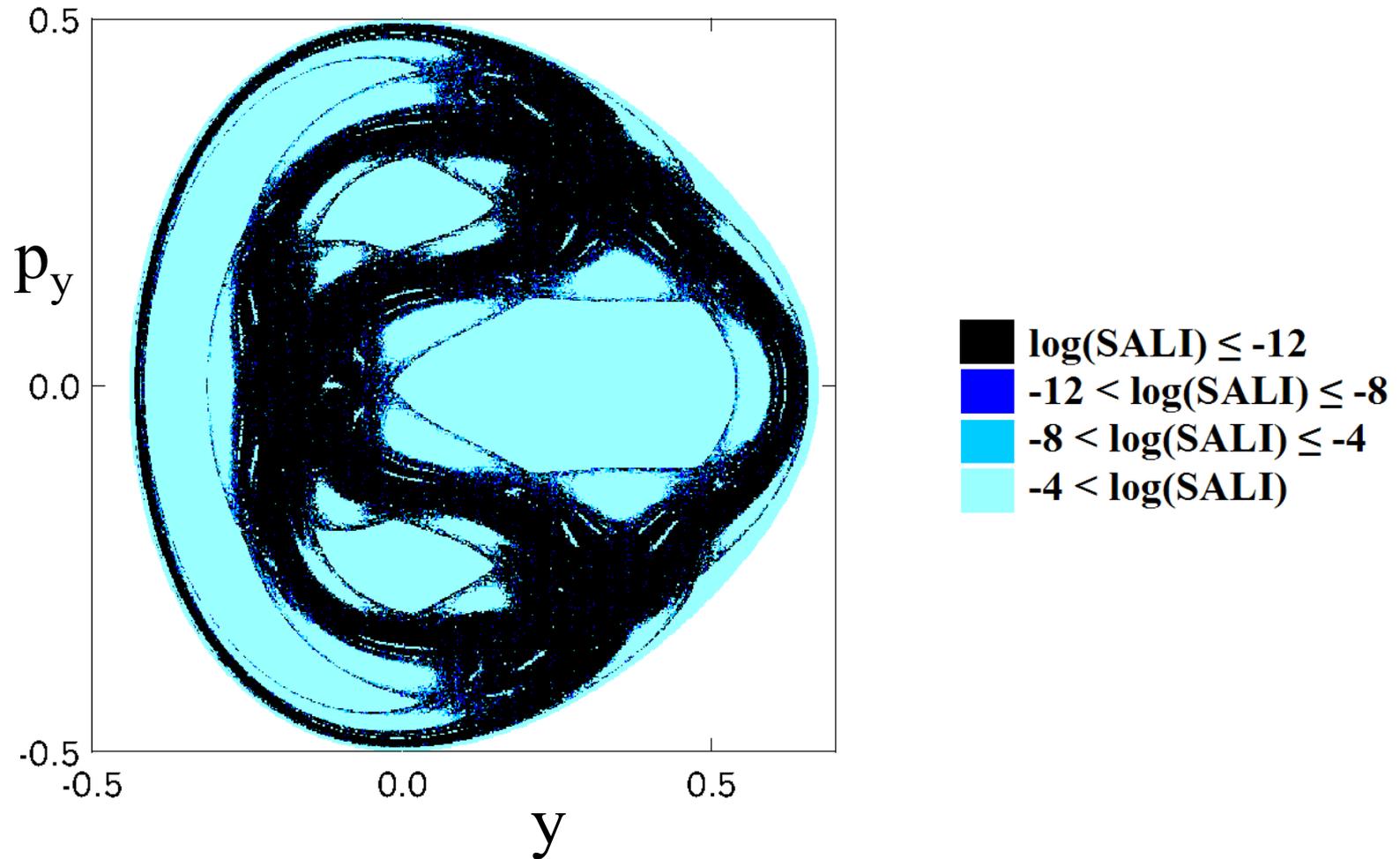
Regular orbit, $x=0, y=0.55, p_x=0.2417, p_y=0$

Chaotic orbit, $x=0, y=-0.016, p_x=0.49974, p_y=0$

Chaotic orbit, $x=0, y=-0.01344, p_x=0.49982, p_y=0$



SALI – Hénon-Heiles system



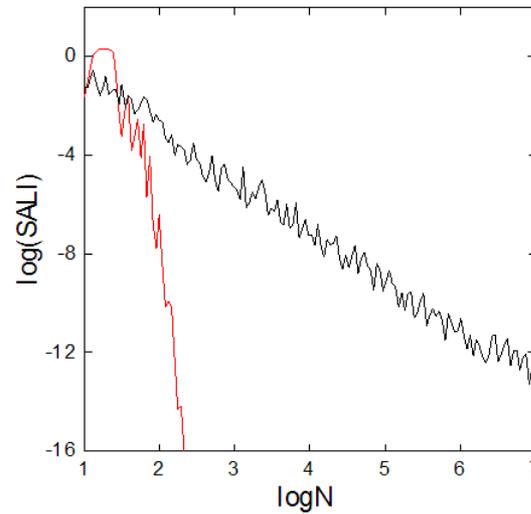
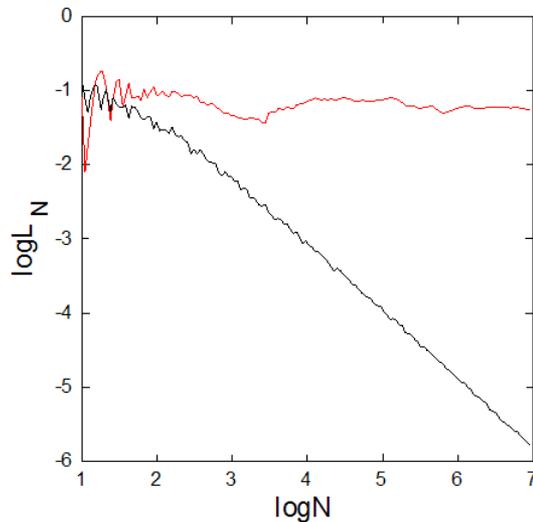
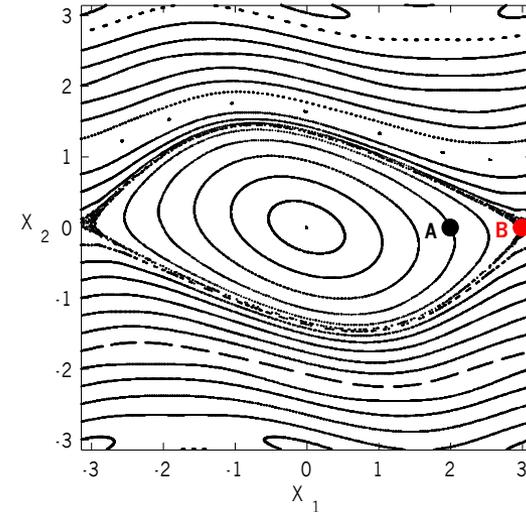
Applications – 2D map

$$\begin{aligned}x_1' &= x_1 + x_2 \\x_2' &= x_2 - \nu \sin(x_1 + x_2)\end{aligned}\quad (\text{mod } 2\pi)$$

For $\nu=0.5$ we consider the orbits:

regular orbit A with initial conditions $x_1=2, x_2=0$.

chaotic orbit B with initial conditions $x_1=3, x_2=0$.



Behavior of the SALI

2D maps

SALI $\rightarrow 0$ both for regular and chaotic orbits

following, however, completely different time rates which allows us to distinguish between the two cases.

Hamiltonian flows and multidimensional maps

SALI $\rightarrow 0$ for chaotic orbits

SALI \rightarrow constant $\neq 0$ for regular orbits

Using LDs to quantify chaos

We consider orbits on a finite grid of an $n(\geq 1)$ -dimensional subspace of the $N(\geq n)$ -dimensional phase space of a dynamical system and their LDs.

Any non-boundary point x in this subspace has $2n$ nearest neighbors

$$y_i^\pm = x \pm \sigma^{(i)} e^{(i)}, \quad i = 1, 2, \dots, n,$$

where $e^{(i)}$ is the i th usual basis vector in \mathbb{R}^n and $\sigma^{(i)}$ is the distance between successive grid points in this direction.

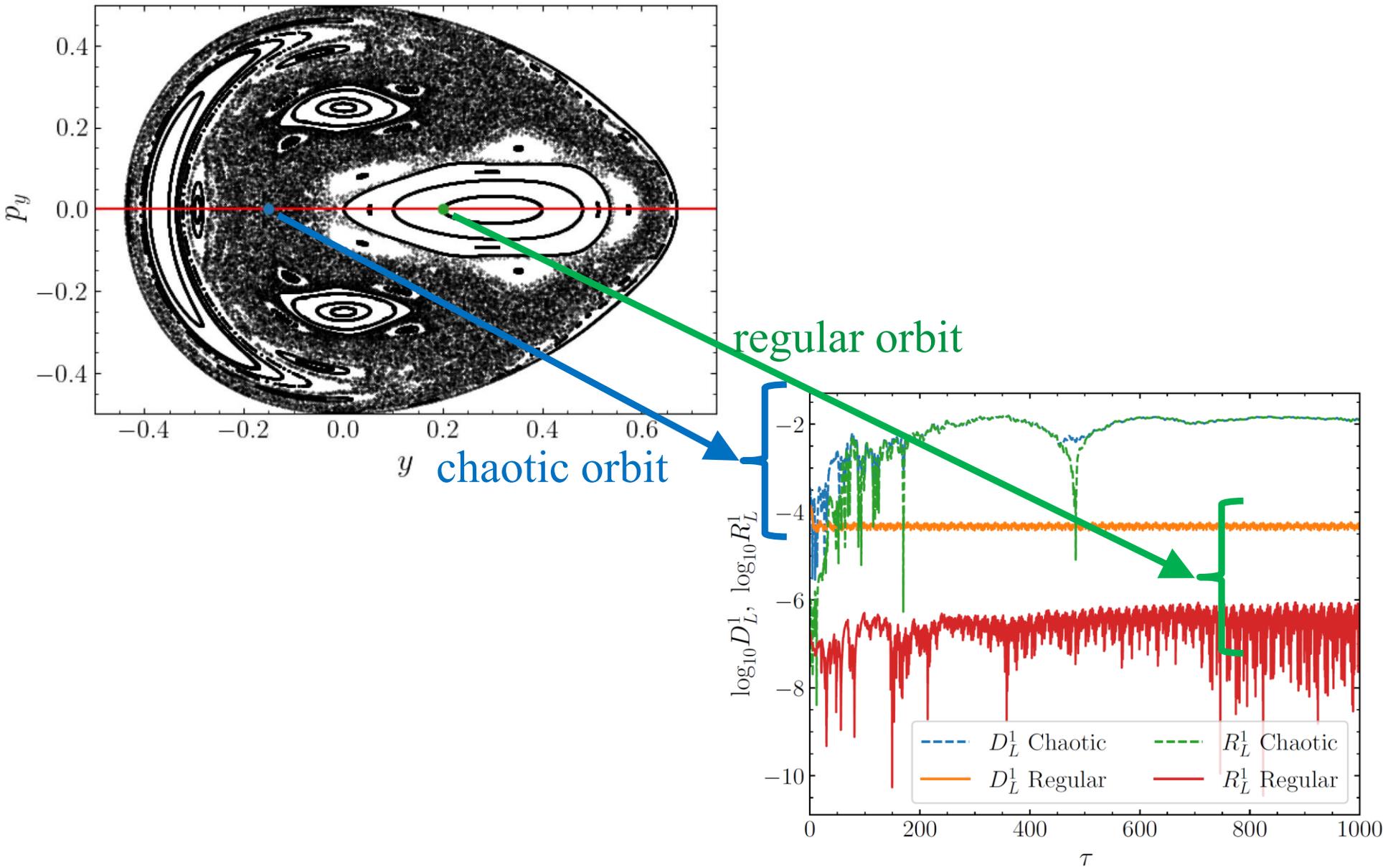
The **difference** D_L^n of neighboring orbits' LDs:

$$D_L^n(x) = \frac{1}{2n} \sum_{i=1}^n \frac{|LD^f(x) - LD^f(y_i^+)| + |LD^f(x) - LD^f(y_i^-)|}{LD^f(x)}.$$

The **ratio** R_L^n of neighboring orbits' LDs:

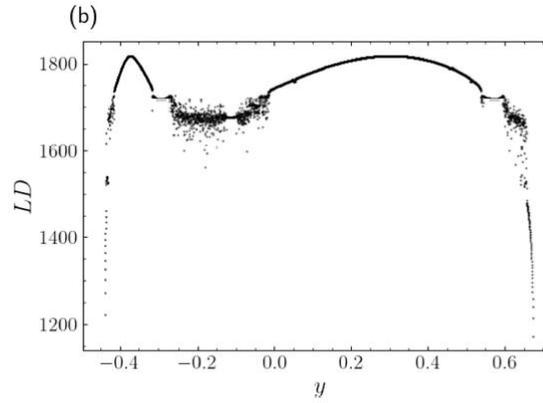
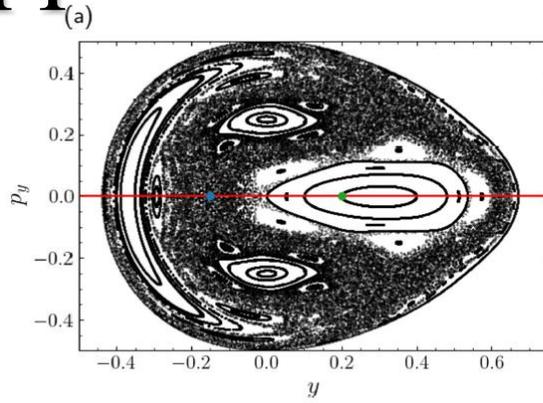
$$R_L^n(x) = \left| 1 - \frac{1}{2n} \sum_{i=1}^n \frac{LD^f(y_i^+) + LD^f(y_i^-)}{LD^f(x)} \right|.$$

Application: Hénon-Heiles system



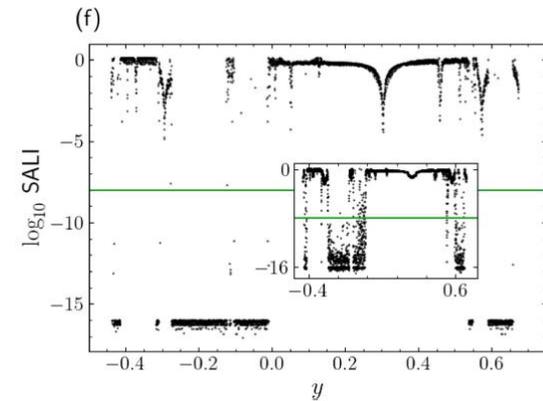
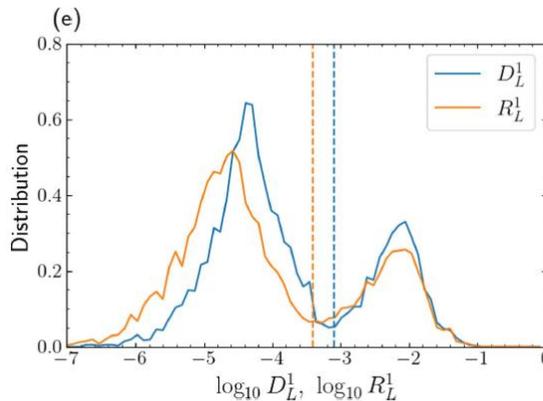
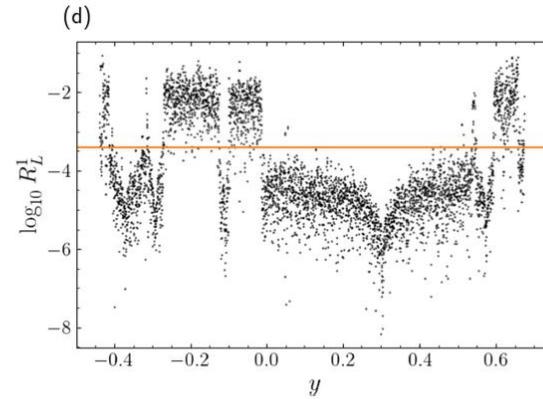
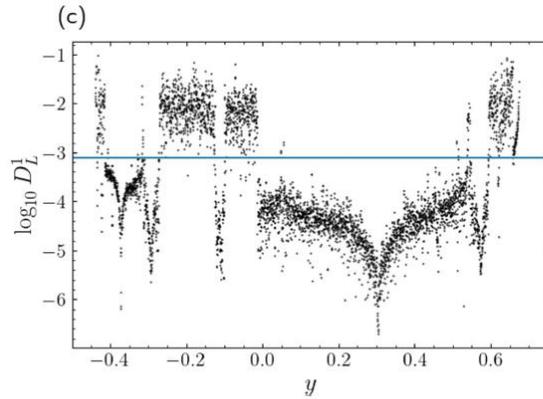
Application: Hénon-Heiles system

H=1/8



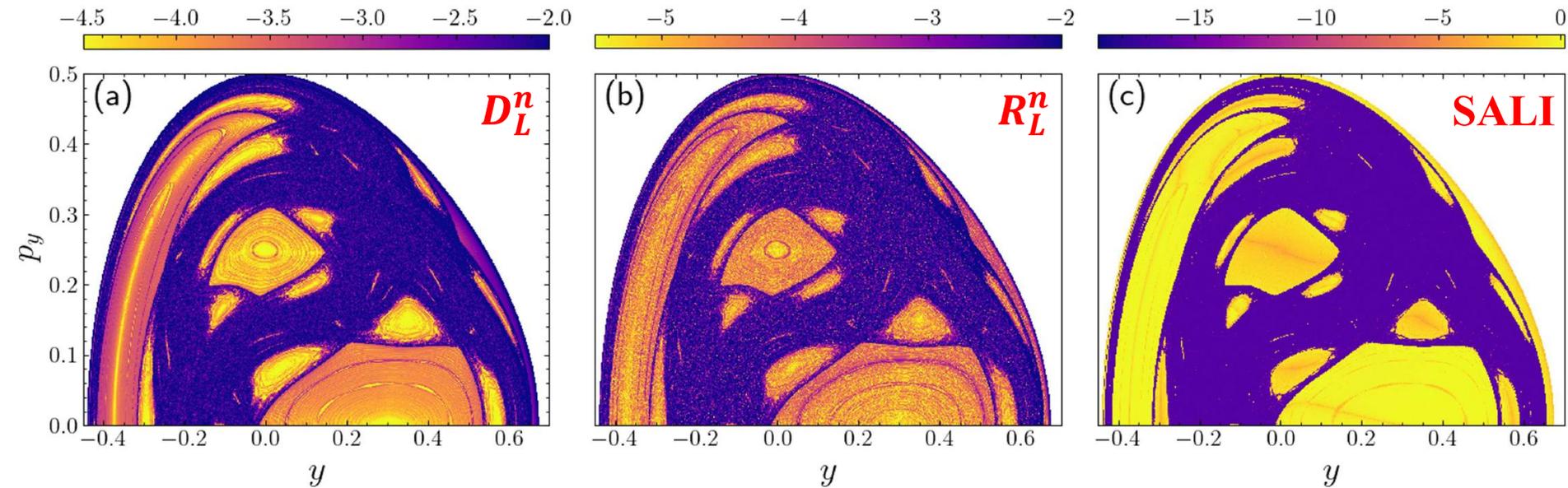
Variation of LDs with regard to initial conditions.
regular regions: smooth
chaotic regions: erratic
[also see Montes et al., Commun. Nonlin. Sci. Num. Simul. (2021)]

LDs for $\tau=10^3$

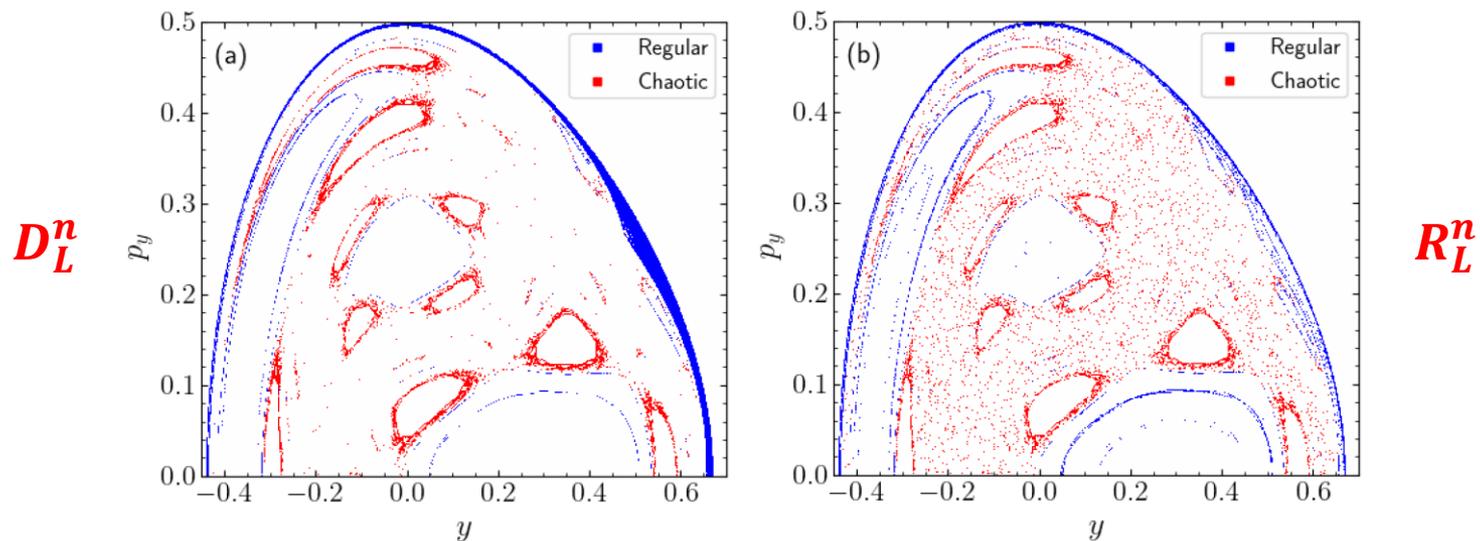


SALI for $\tau=10^6$
(inset $\tau=10^3$)

Application: Hénon-Heiles system



Misclassified orbits (< 10%)



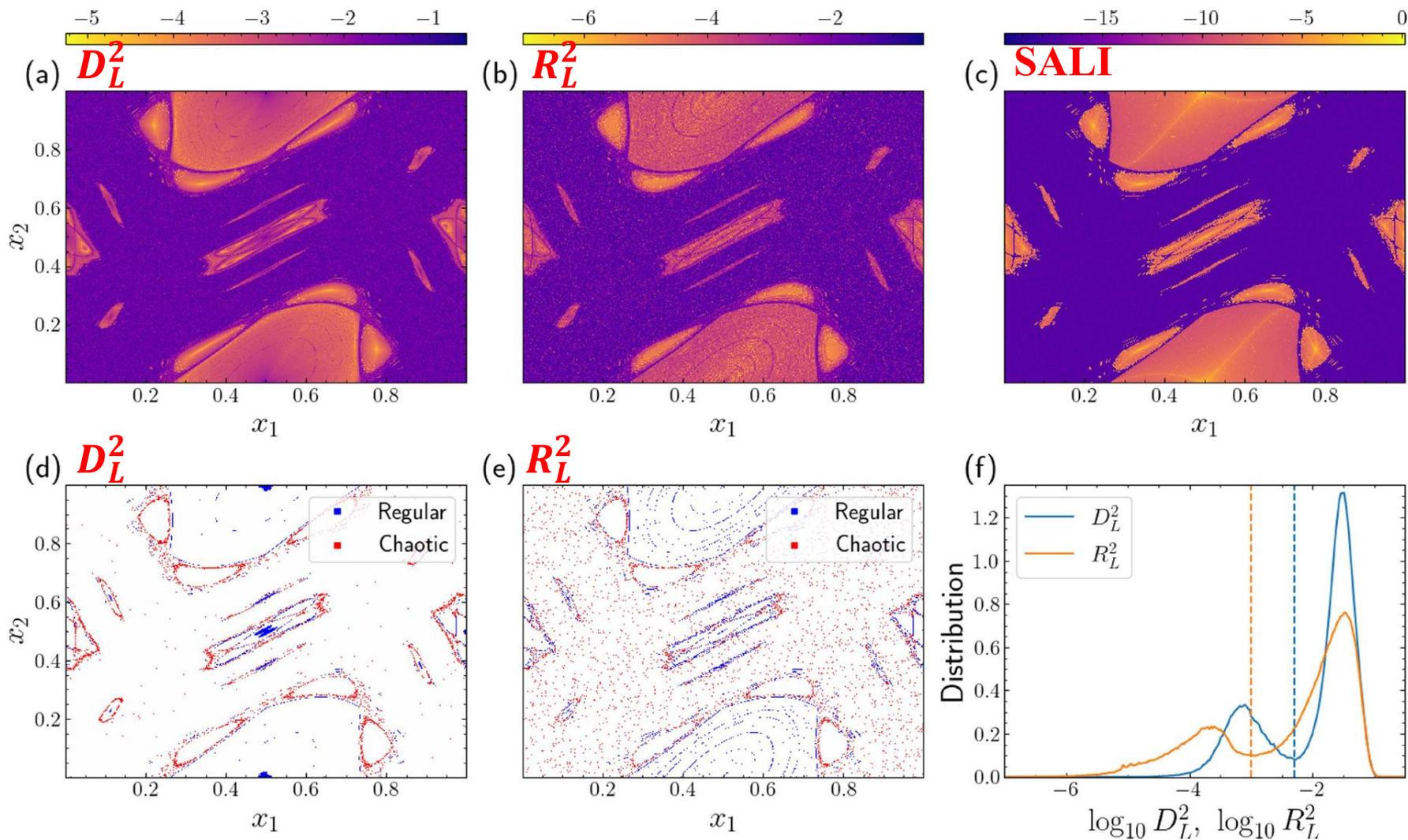
Application: 2D Standard map

$$\begin{aligned} x'_1 &= x_1 + x'_2 \\ x'_2 &= x_2 + \frac{K}{2\pi} \sin(2\pi x_1) \pmod{1} \end{aligned}$$

We set $K = 1.5$

Thresholds: $\log_{10} D_L^2 = -2.3$, $\log_{10} R_L^2 = -3$ ($T = 10^3$)

$\log_{10} \text{SALI} = -12$ ($T = 10^5$)

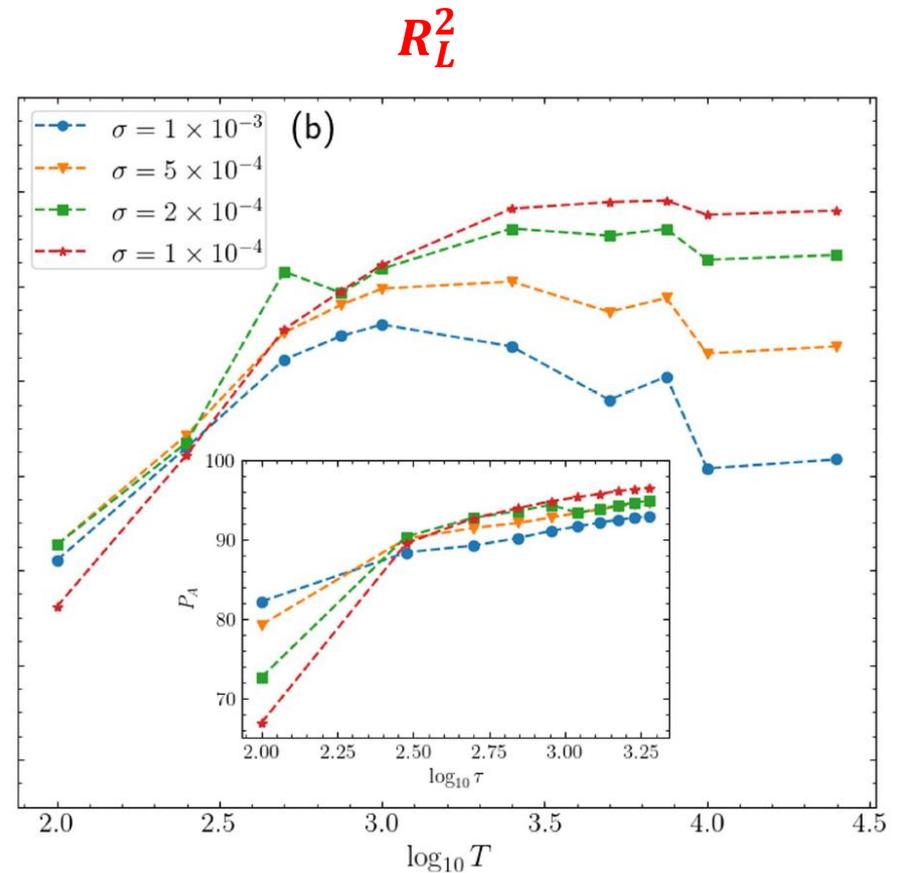
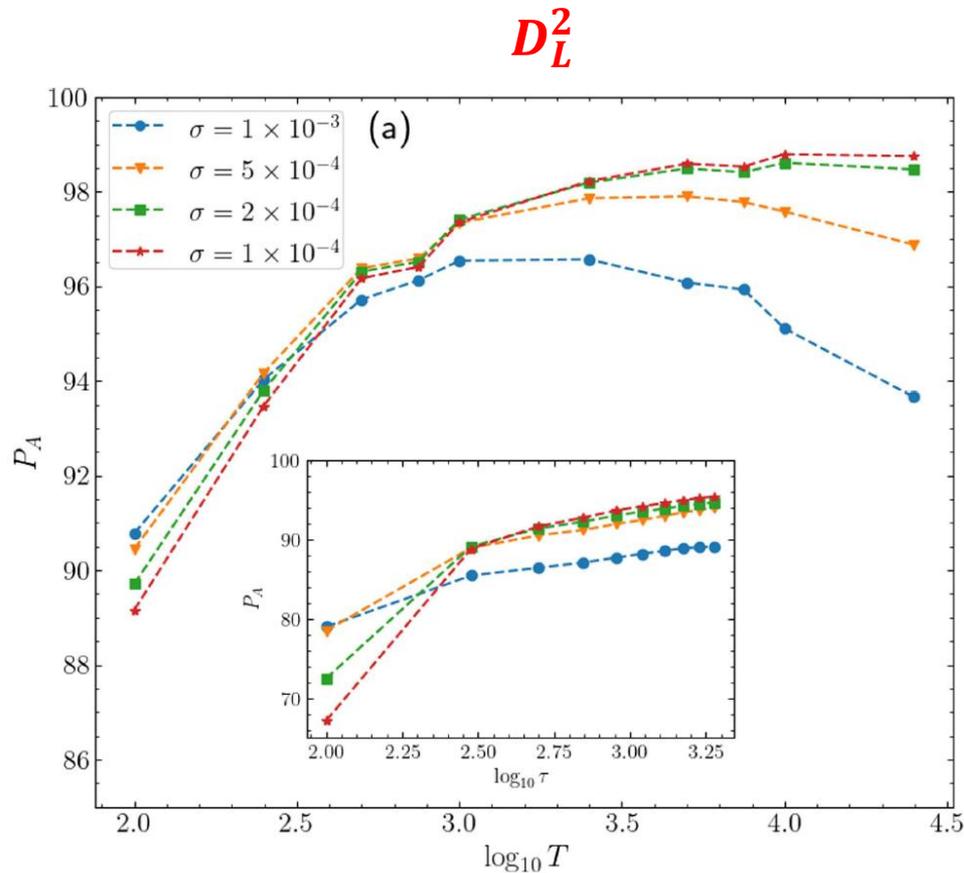


Effect of grid spacing (σ) and final integration time (T, τ)

P_A : percentage of correctly characterized orbits

Main plots: 2D Standard map

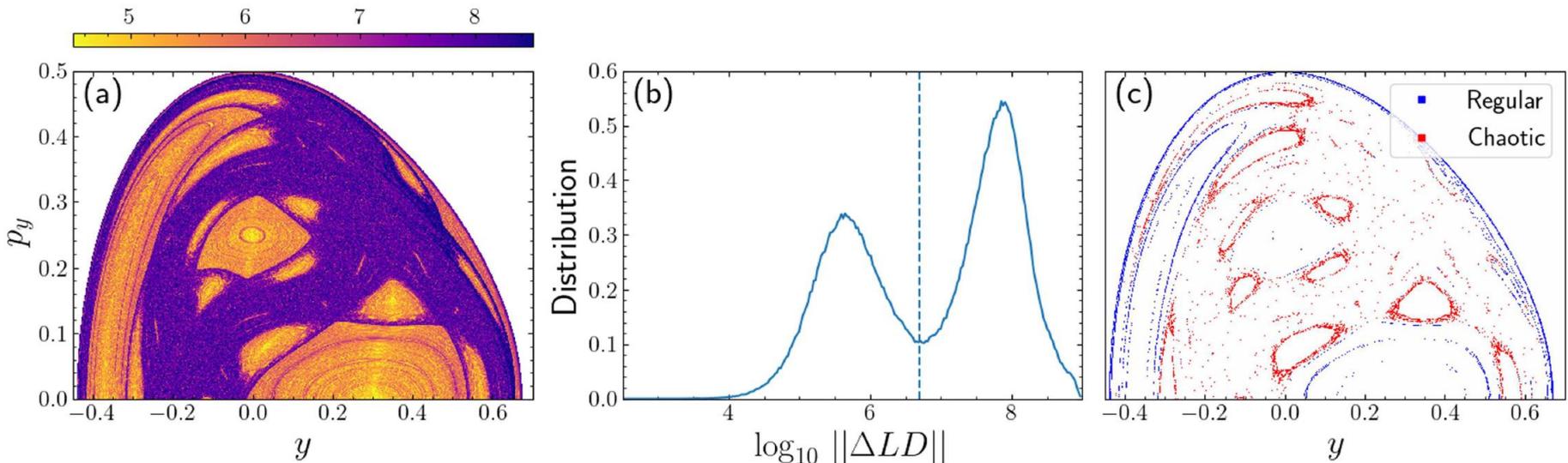
Insets: Hénon-Heiles system



Application: Hénon-Heiles system

A quantity related to **the second spatial derivative of the LDs** was introduced in Daquin et al., Physica D (2022) and was used in Hillebrand et al., Chaos (2022):

$$\|\Delta LD\|(x) = \left| \frac{LD^f(y_i^+) - 2LD^f(x) + LD^f(y_i^-)}{\sigma^2} \right|.$$

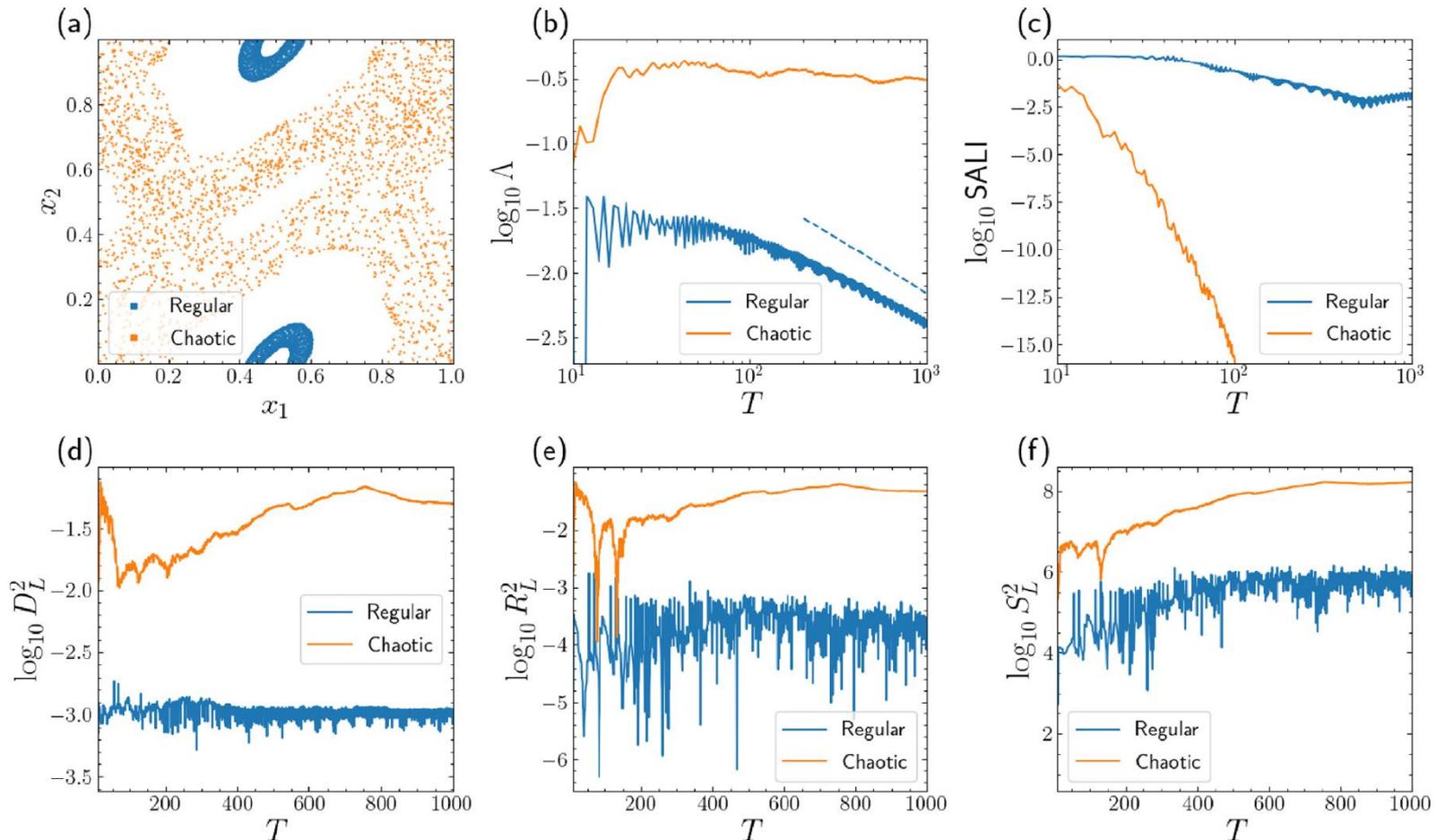


In Zimmer et al., Physica D (2023) it was modified to:

$$S_L^n(x) = \frac{1}{n} \sum_{i=1}^n \left| \frac{LD^f(y_i^+) - 2LD^f(x) + LD^f(y_i^-)}{(\sigma^{(i)})^2} \right|.$$

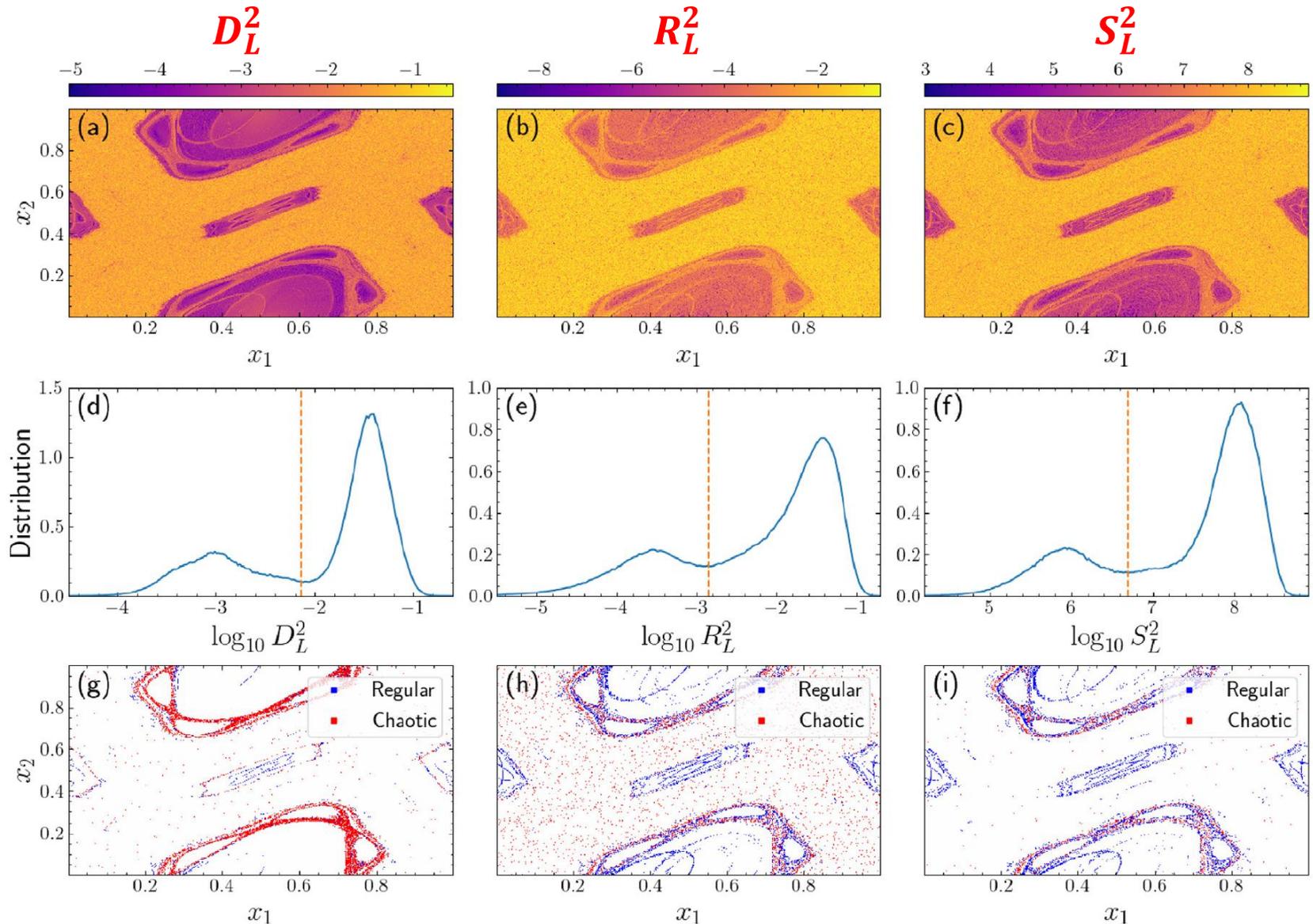
Application: 4D Standard map

$$\begin{aligned}x'_1 &= x_1 + x'_2 \\x'_2 &= x_2 + \frac{K}{2\pi} \sin(2\pi x_1) - \frac{B}{2\pi} \sin[2\pi(x_3 - x_1)] \\x'_3 &= x_3 + x'_4 \\x'_4 &= x_4 + \frac{K}{2\pi} \sin(2\pi x_3) - \frac{B}{2\pi} \sin[2\pi(x_1 - x_3)]\end{aligned} \quad (\text{mod } 1)$$



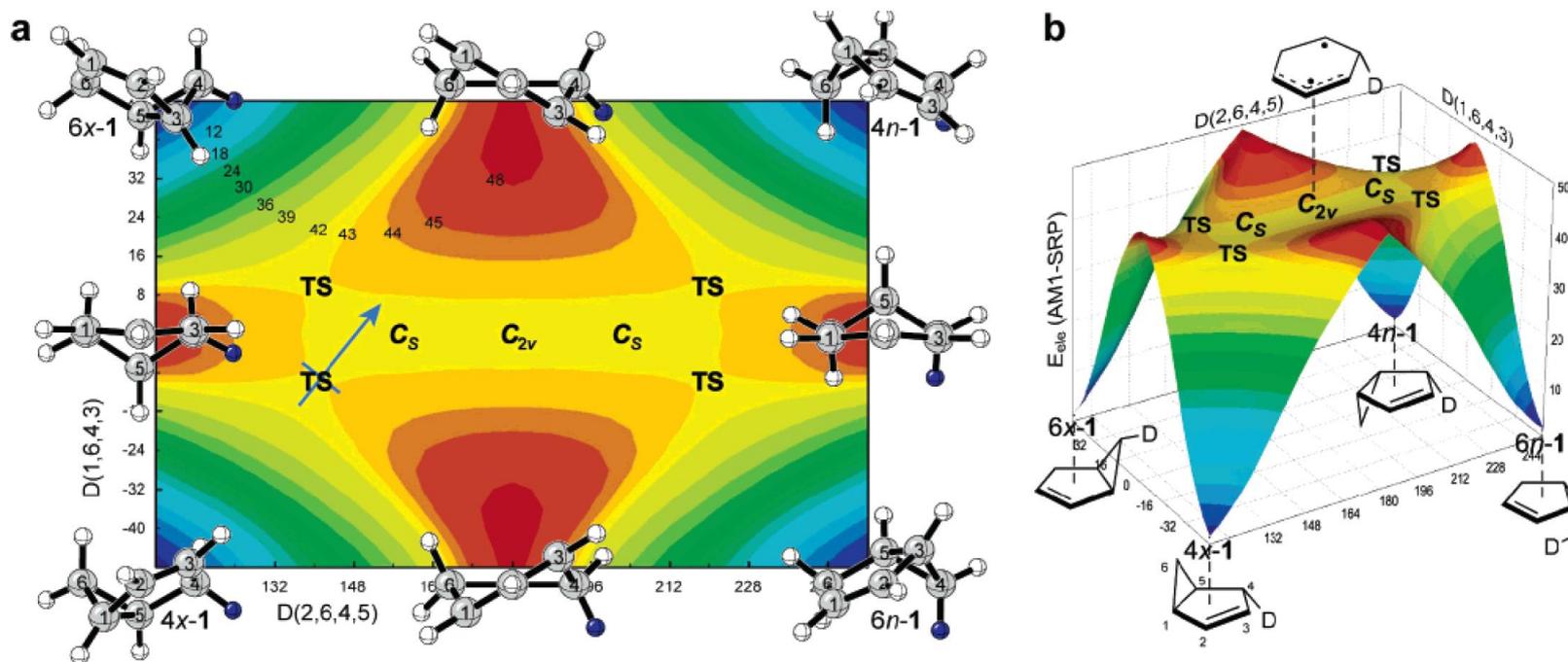
Application: 4D Standard map

2D subspace (x_1, x_2) with $x_3 = 0.54, x_4 = 0.01$ for $K = 1.5, B = 0.05$ and $T = 10^3$



The caldera potential energy surface

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



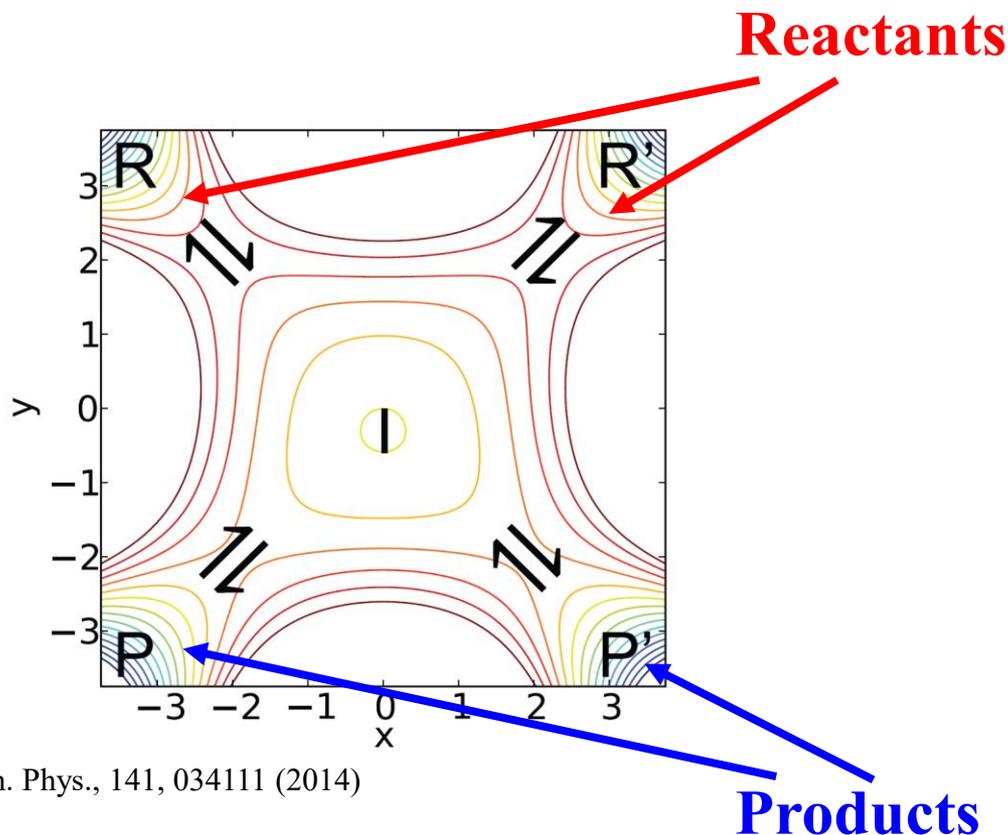
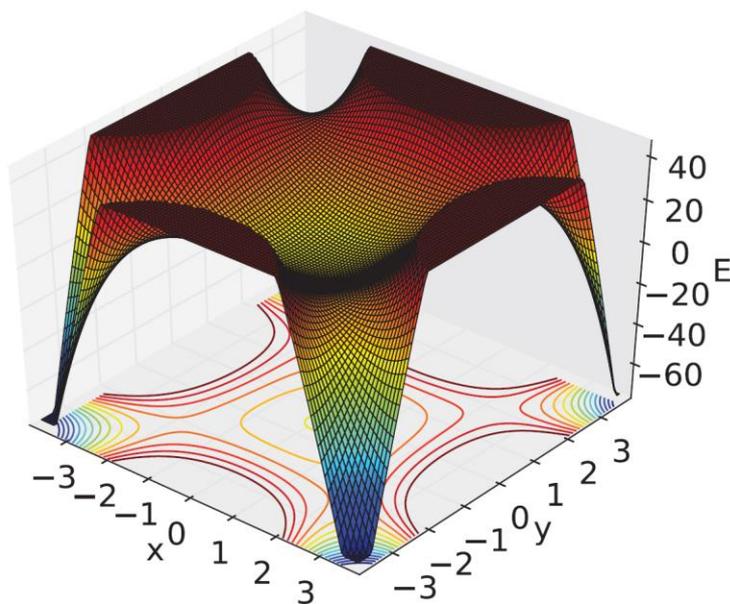
From Doubleday, Suhrada, Houk., J. Am. Chem. Soc., 128, 90 (2006)

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):

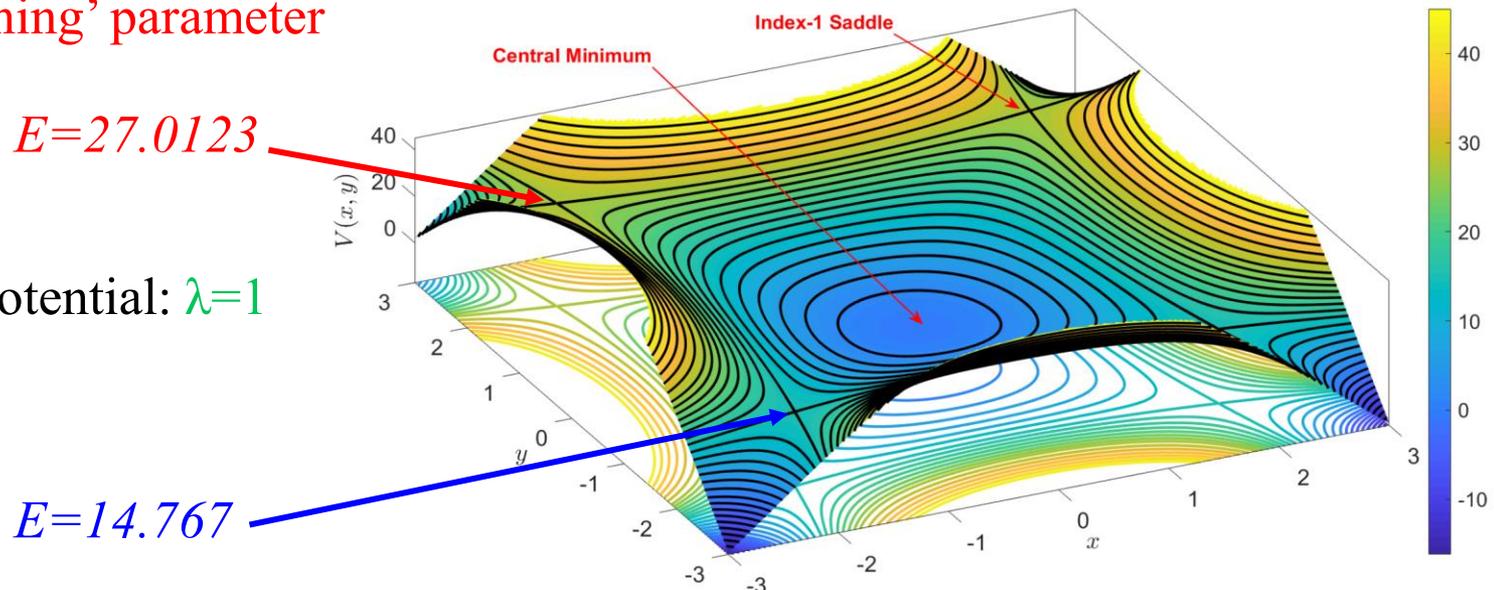
$$H(x, y, p_x, p_y) = \frac{1}{2} (p_x^2 + p_y^2) + V(x, y)$$

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

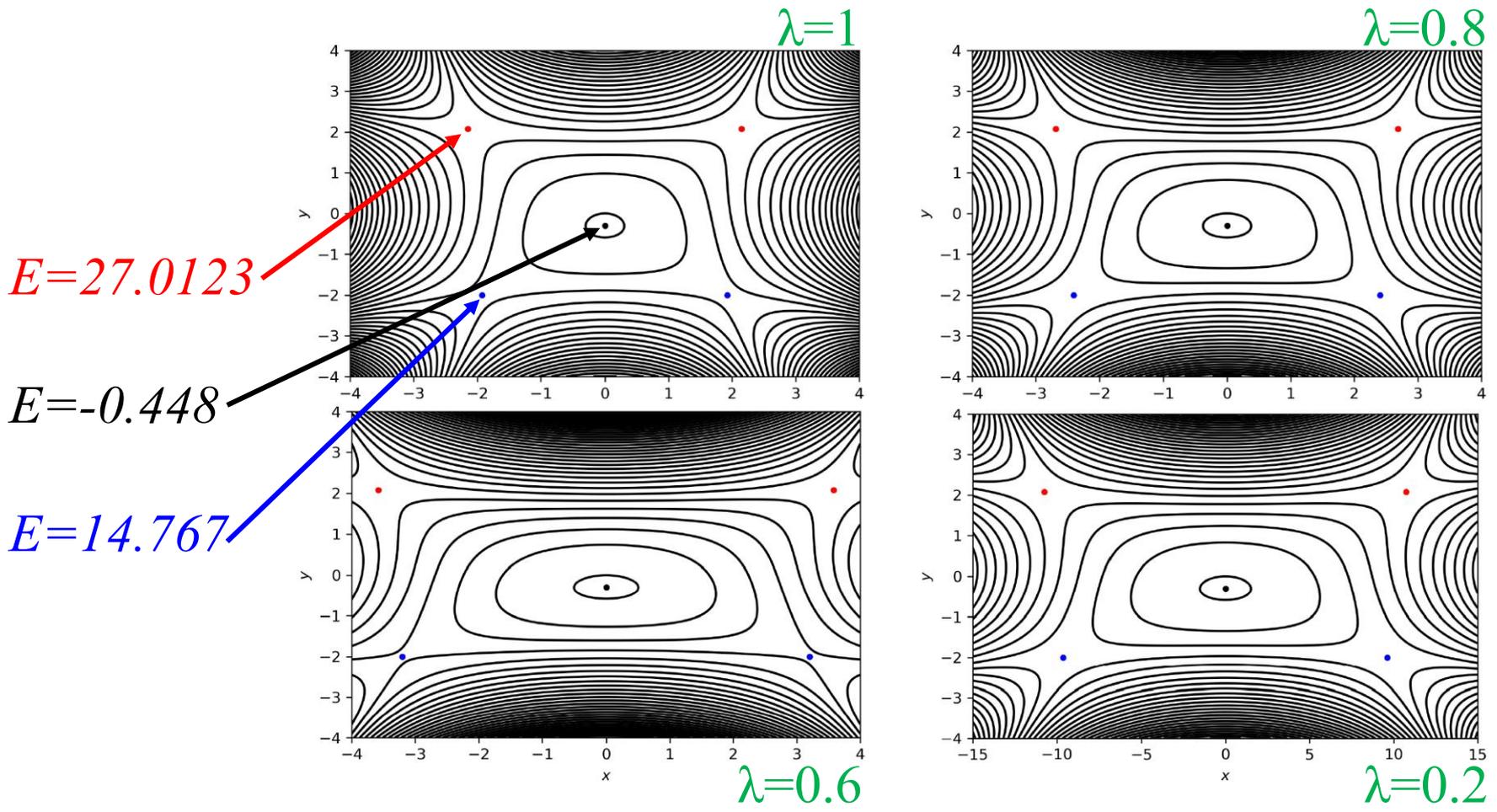
Symmetric potential: $\lambda=1$



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, $0 < \lambda < 1$)



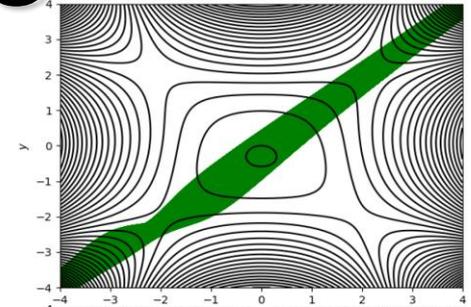
Dynamical matching

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.

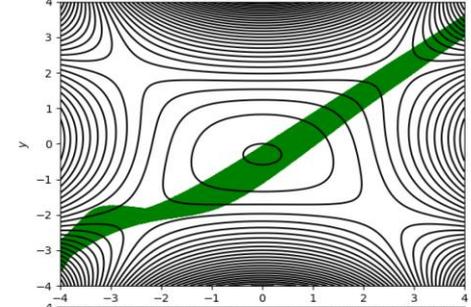
Critical value for the breaking of dynamical matching: $\lambda = 0.778$ (Katsanikas et al., Int. J. Bifurcat. Chaos, 2020)

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.**

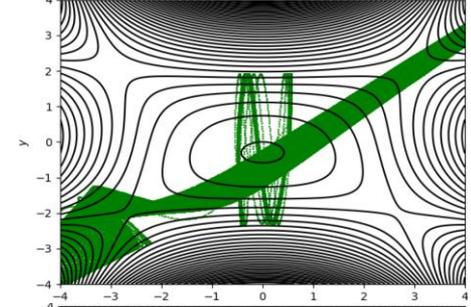
$$\lambda=1$$



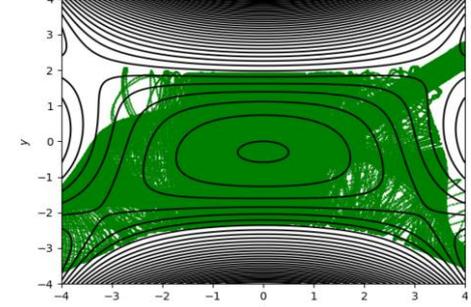
$$\lambda=0.8$$



$$\lambda=0.72$$



$$\lambda=0.6$$



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):

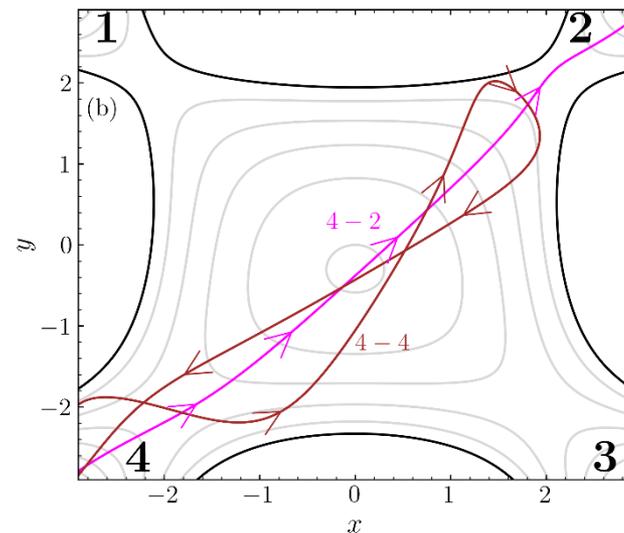
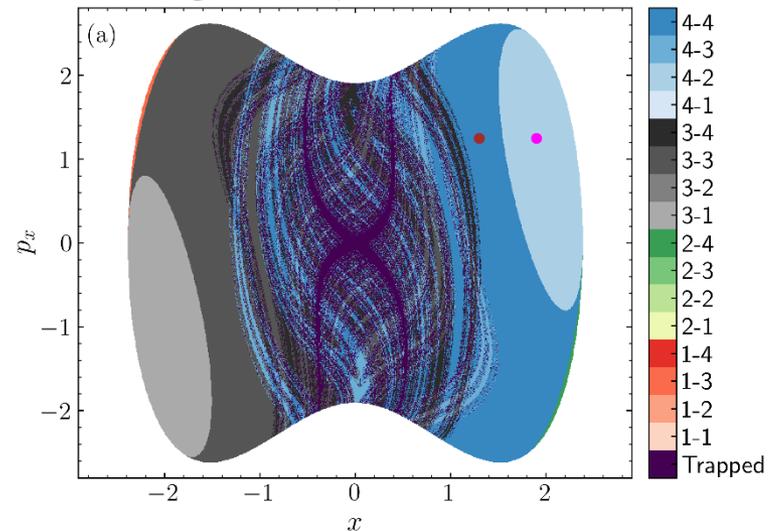
$$y = 1.88409, \quad p_y > 0,$$

$$E = 29.$$

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

Escape condition: $|y| > 6$

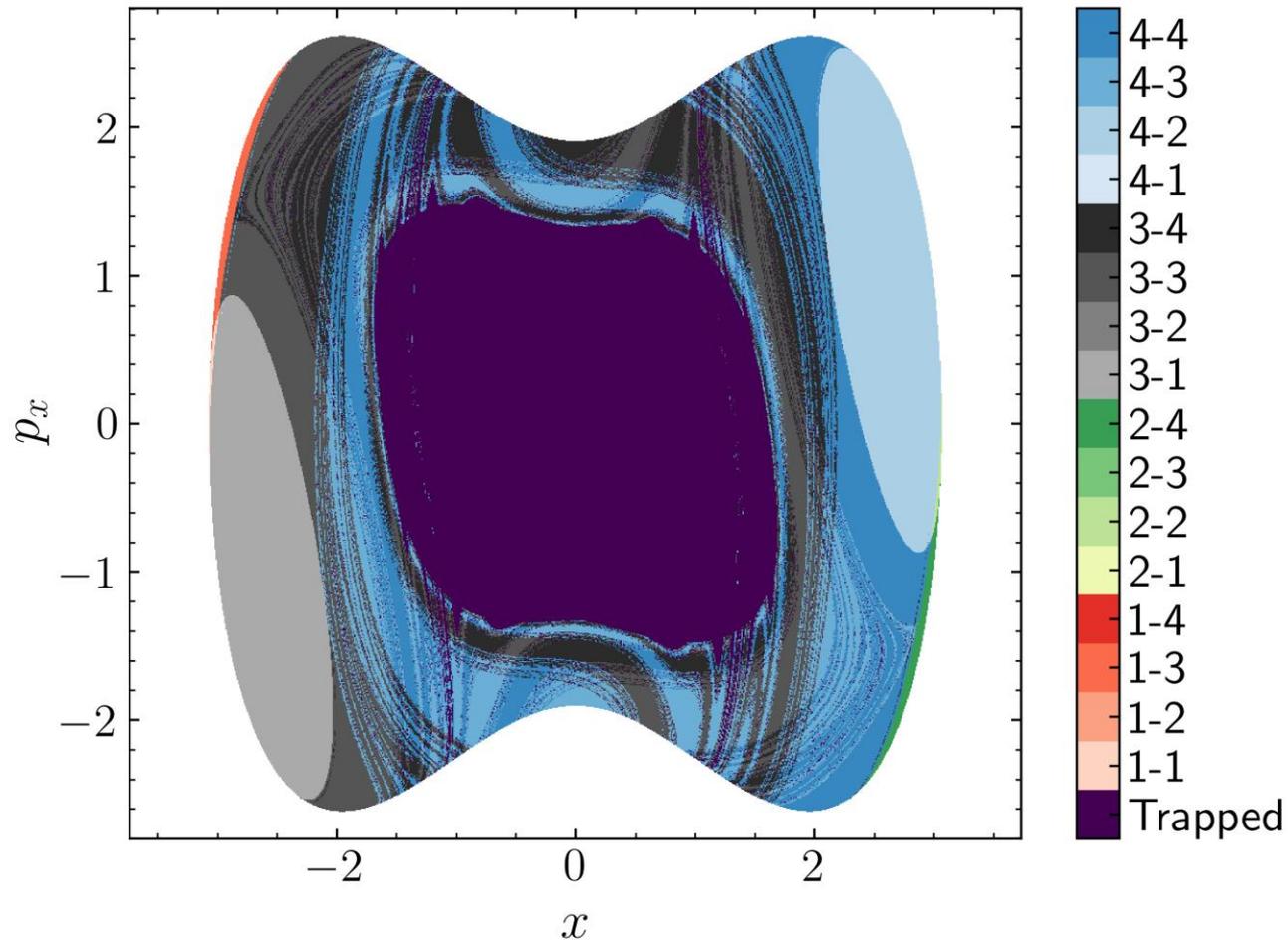
Trapped: an orbit does not escape in either the forward or backward integration.



The origin fate map (OFM)

Stretched potential: $\lambda=0.778$

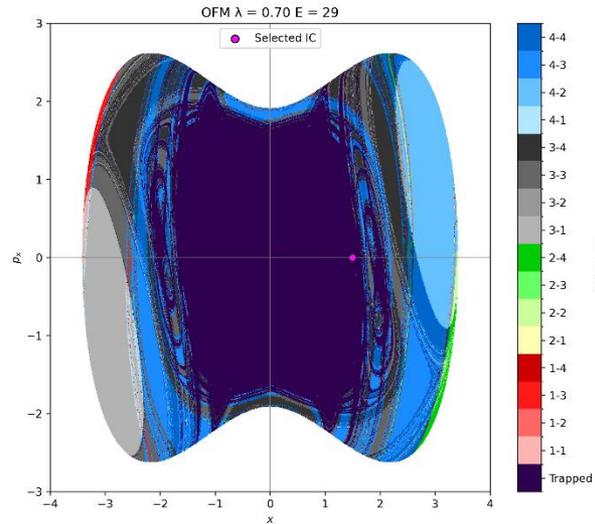
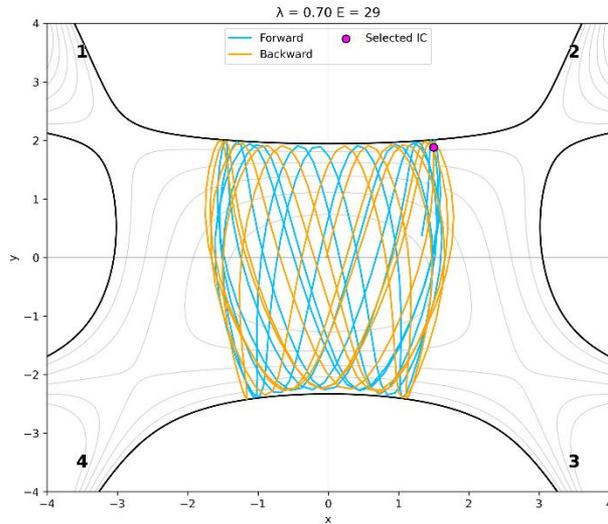
PSS: $y = 1.88409$, $p_y > 0$, $E = 29$. Integration time: $\tau = 20$ time units.



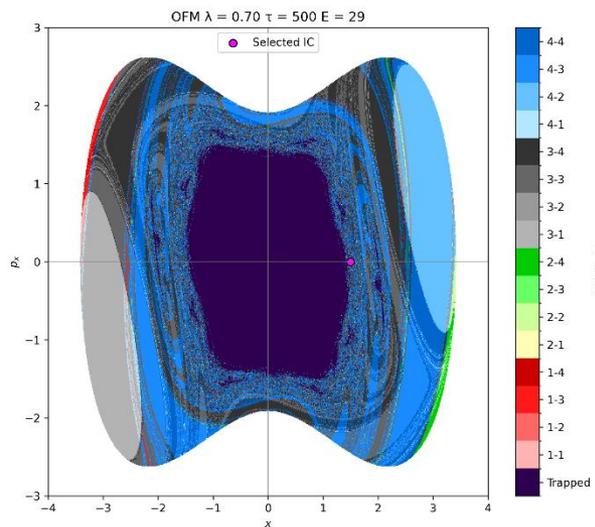
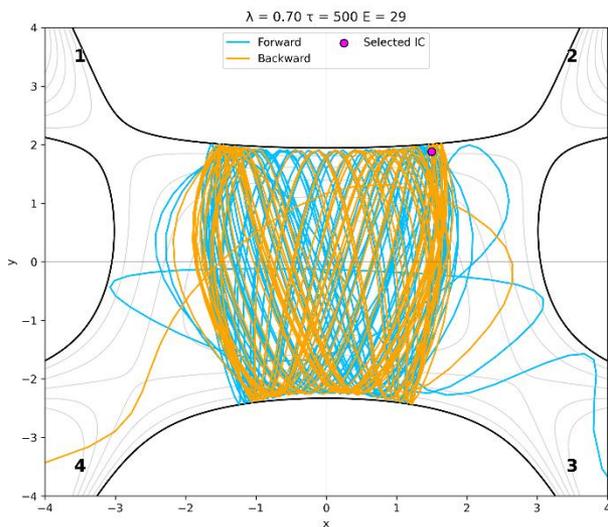
The origin fate map (OFM)

Stretched potential: $\lambda=0.7$

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



$\tau = 20$

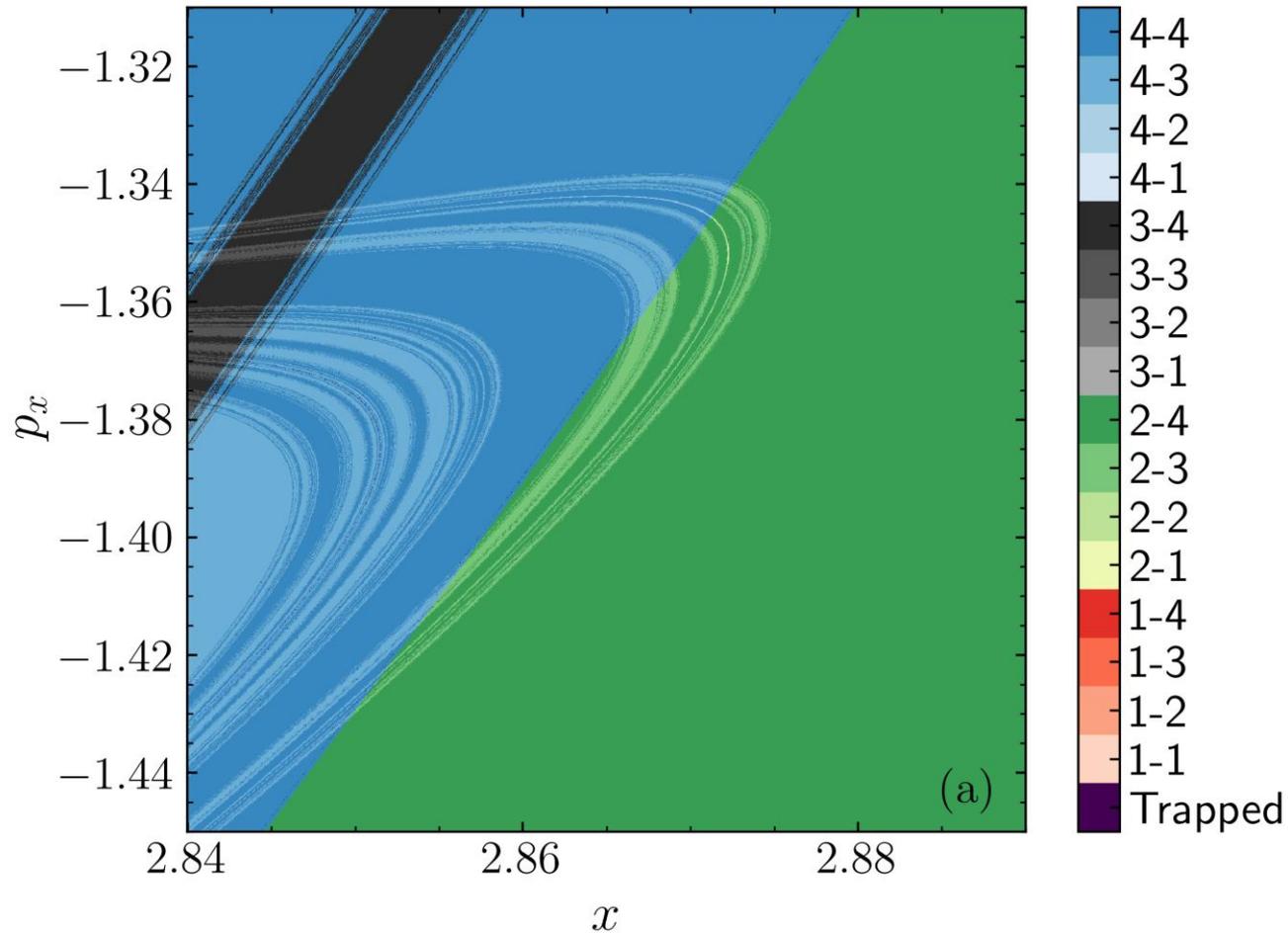


$\tau = 500$

OFM and manifold dynamics

Stretched potential: $\lambda=0.778$

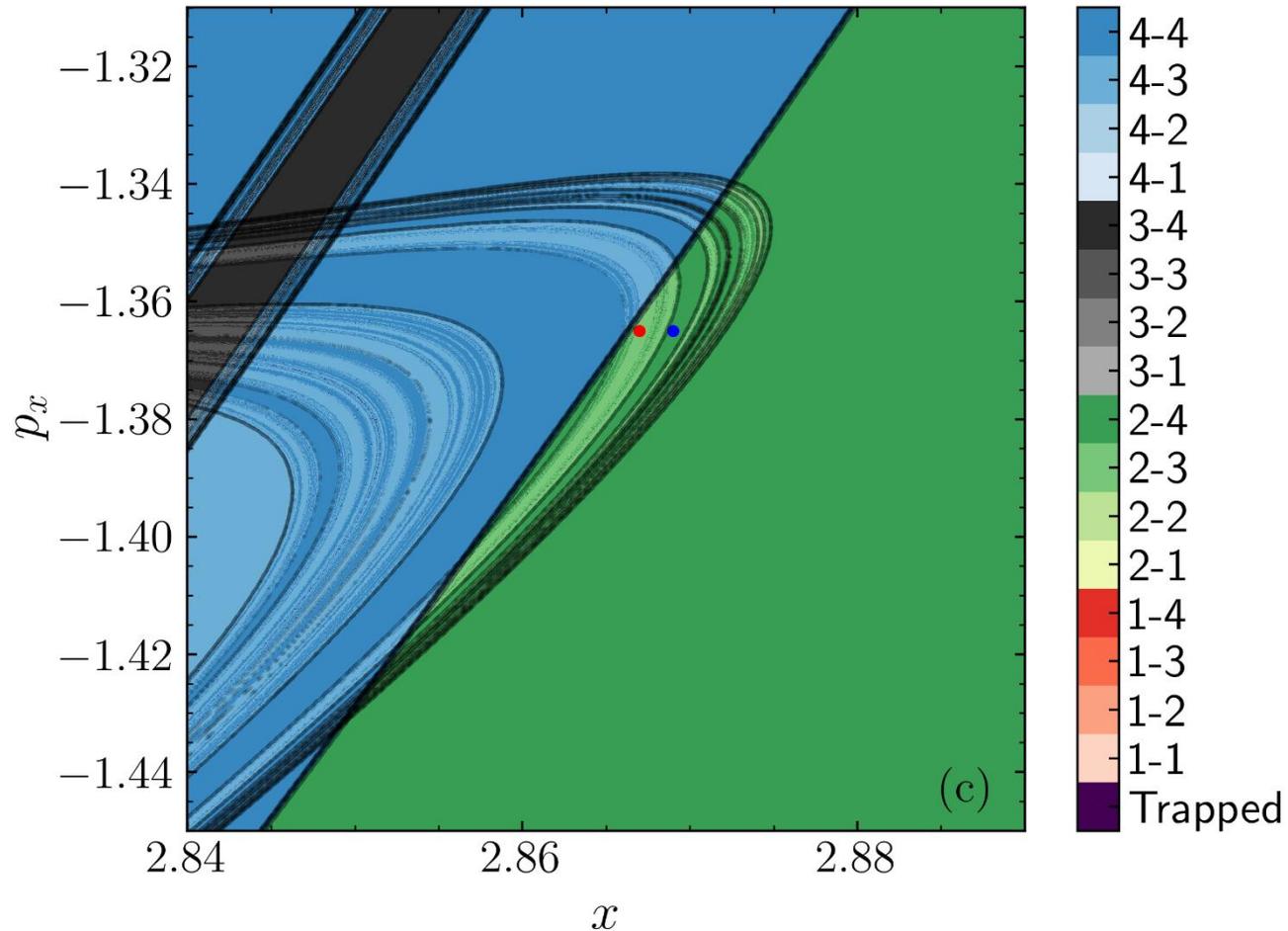
PSS: $y = 1.88409$, $p_y > 0$, $E = 29$. Integration time: $\tau = 20$ time units.



OFM and manifold dynamics

Stretched potential: $\lambda=0.778$

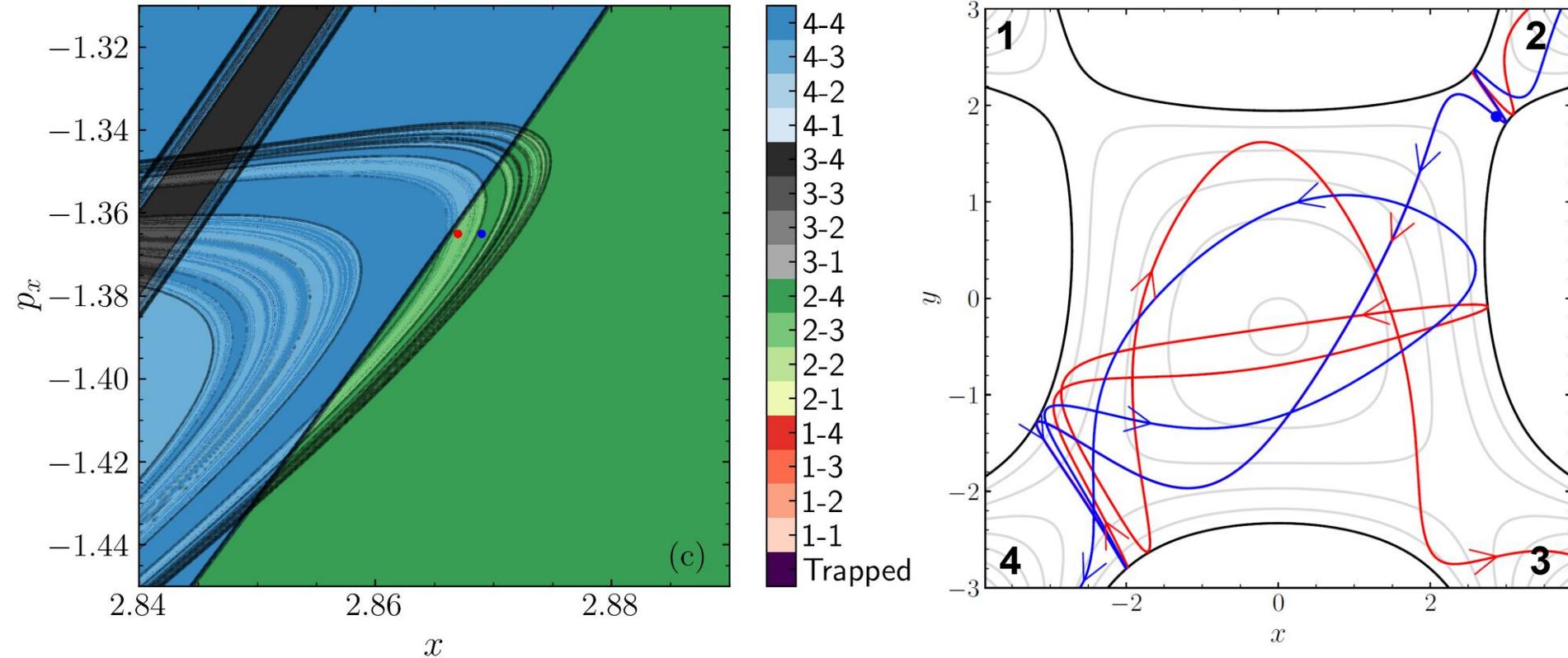
PSS: $y = 1.88409$, $p_y > 0$, $E = 29$. Integration time: $\tau = 20$ time units.



OFM and manifold dynamics

Stretched potential: $\lambda=0.778$

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



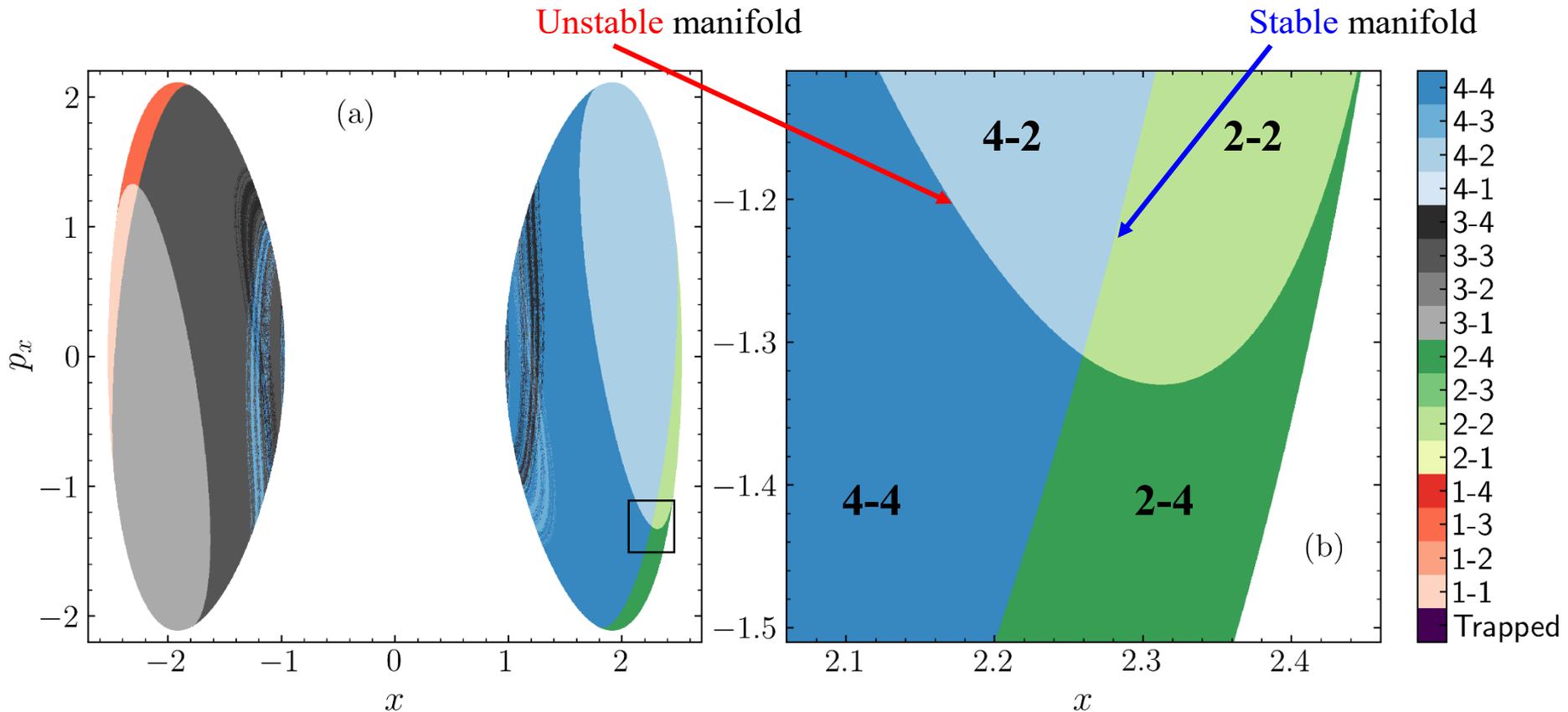
$$(x, y, p_x, p_y) = (2.876, 1.88409, -1.365, 0.86563646)$$

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

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

Summary I

- ✓ We introduced and successfully implemented computationally efficient ways to **effectively identify chaos** in conservative dynamical systems **from the values of LDs at neighboring initial conditions**.
- ✓ From the distributions of the indices' values we determine appropriate **threshold values**, which allow the characterization of orbits as regular or chaotic.
- ✓ All indices **faced problems** in correctly revealing the nature of some orbits mainly **at the borders of stability islands**.
- ✓ All indices show **overall very good performance**, as their classifications are in accordance with the ones obtained by **the SALI (which is a very efficient and accurate chaos indicator)** at a level of at least 90% agreement.
- ✓ **Advantages:**
 - **Easy to compute** (actually only the forward LDs are needed).
 - **No need to know and to integrate the variational equations.**

Summary II

- ✓ 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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