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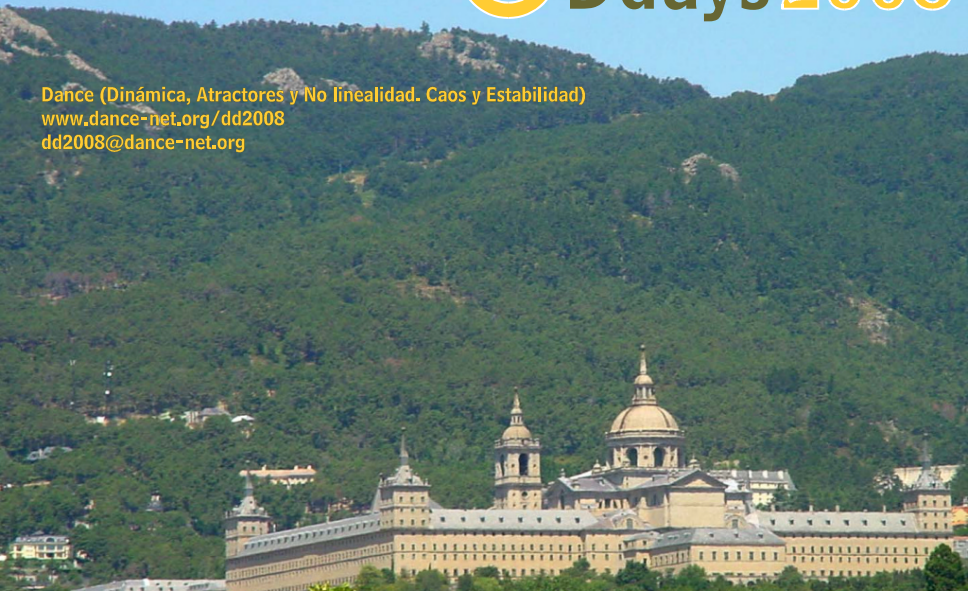
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# The role of hyperbolic invariant objects: From Arnold diffusion to biological clocks

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# Outline

- 1 Arnold diffusion for a priori unstable Hamiltonian Systems
  - Arnold diffusion
  - Main result
  - Sketch of the Proof
- 2 Fast numerical algorithms to compute invariant tori in Hamil. Systems
- 3 A computational and geometric approach to PRC and PRS

# Part I: Arnold diffusion for a priori unstable Hamiltonian Systems

# Arnold diffusion

- Nearly-integrable Hamiltonian systems of  $n$ -degrees of freedom

$$H(I, \varphi) = H_0(I) + \epsilon H_1(I, \varphi)$$

where  $(I, \varphi) \in \mathbb{R}^n \times \mathbb{T}^n$ .

- For  $\epsilon = 0$  all the trajectories lie on an invariant tori  $I = ct$ . All trajectories are **stable**.
- KAM theorem**. Under a suitable non-degeneracy condition the  $n$ -dimensional invariant tori  $I = ct$  with Diophantine frequency  $\omega(I)$  survive, with some deformation, for  $\epsilon$  small enough. Provides stability for  $n \leq 2$ .
- Question**: What happens for the trajectories which do not lie on the invariant tori, for  $n > 2$ ? Do there exist **unstable orbits**, that is, orbits whose action variable (slow variable) experiences a drift of order 1?

## Main contributions in Arnold diffusion

- Arnold'64 (Example of a Hamiltonian of  $2+1/2$  degrees of freedom with 2 parameters).
- A priori unstable case (the unperturbed Hamiltonian  $H_0$  presents hyperbolicity: integrable pendulum) without gaps (non-generic perturbation  $H_1$ ): Chierchia and Gallavotti '94 '98, Berti, Biasco, Bolle '02 '03 (with time estimates).
- A priori unstable case overcoming the large gap problem: Cheng and Yan '04 (variational methods), Treschev '04 (separatrix map), Delshams, de la Llave and Seara '03 '06 (Geometric methods), de la Llave and Gidea '06 (Topological methods).

Goal: Generalize the result in [DLS06] for generic perturbations.

[DLS06] A. Delshams, R. de la Llave and T.M. Seara. A geometric mechanism for diffusion in Hamiltonian systems overcoming the large gap problem: heuristics and rigorous verification on a model. *Mem. Amer. Math. Soc.*, 179 (844), 2006.

# Instability for a priori unstable Hamiltonian systems

We consider a  $2\pi$ -periodic in time perturbation of a **pendulum** and a **rotor** described by the non-autonomous Hamiltonian of 2+1/2-dof,

$$\begin{aligned} H_\epsilon(p, q, I, \varphi, t) &= H_0(p, q, I) + \epsilon h(p, q, I, \varphi, t; \epsilon) \\ &= P_\pm(p, q) + \frac{1}{2}I^2 + \epsilon h(p, q, I, \varphi, t; \epsilon) \end{aligned} \quad (1)$$

where  $(p, q, I, \varphi, t) \in (\mathbb{R} \times \mathbb{T})^2 \times \mathbb{T}$  and

$$P_\pm(p, q) = \pm \left( \frac{1}{2}p^2 + V(q) \right) \quad (2)$$

and  $V(q)$  is a  $2\pi$ -periodic function. We will refer to  $P_\pm(p, q)$  as the *pendulum*.

# Main result

## Theorem

Consider the Hamiltonian (1) and that  $V$  and  $h$  are uniformly  $C^{r+2}$  for  $r \geq r_0$ , sufficiently large. Assume,

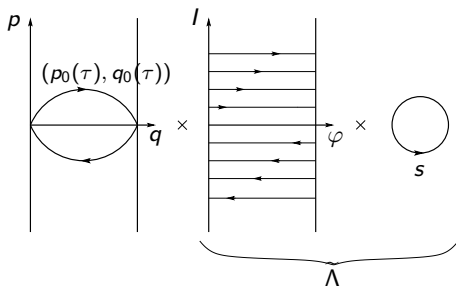
- H1** The potential  $V : \mathbb{T} \rightarrow \mathbb{R}$  has a unique global maximum at  $q = 0$  which is non-degenerate. Denote by  $(q_0(t), p_0(t))$  an orbit of the pendulum  $P_{\pm}(p, q)$  homoclinic to  $(0, 0)$ .
- H2** The *Melnikov potential*, associated to  $h$  (and to the homoclinic orbit  $(p_0, q_0)$ ): satisfies concrete non-degeneracy conditions.
- H3** The perturbation term  $h$  satisfies concrete non-degeneracy conditions.

Then, there is  $\epsilon^* > 0$  such that for  $0 < |\epsilon| < \epsilon^*$ , and for any interval  $[I_-^*, I_+^*] \in (I_-, I_+)$ , there exists a trajectory  $\tilde{x}(t)$  of the system (1) such that for some  $T > 0$ ,

$$I(\tilde{x}(0)) \leq I_-^*; \quad I(\tilde{x}(T)) \geq I_+^*.$$



$$\epsilon = 0$$



- Normally hyperbolic invariant manifold (3D)

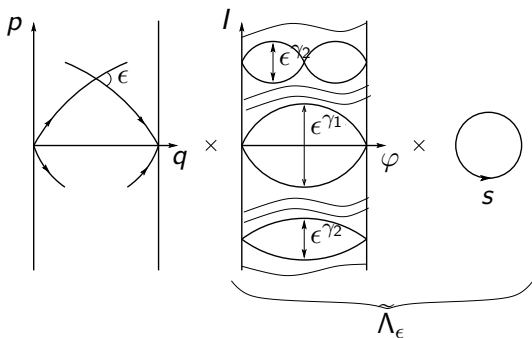
$$\tilde{\Lambda} = \{(0, 0, I, \varphi, s) : (I, \varphi, s) \in \mathbb{R} \times \mathbb{T}^2\}$$

- Invariant manifolds (4D):

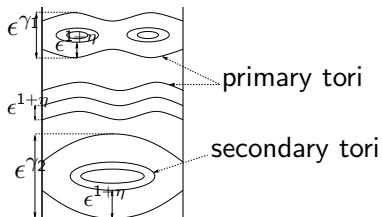
$$W^s \tilde{\Lambda} = W^u \tilde{\Lambda} = \{(p_0(\tau), q_0(\tau), I, \varphi, s) : \tau \in \mathbb{R}, I \in [I_-, I_+], (\varphi, s) \in \mathbb{T}^2\}$$

where  $(p_0(t), q_0(t))$  is an orbit of  $P_{\pm}(p, q)$  homoclinic to  $(0, 0)$ .

$$0 < \epsilon \ll 1$$



- On  $[I_-, I_+]$ ,  $\tilde{\Lambda}$  persists to  $\tilde{\Lambda}_\epsilon$
- $W^s \tilde{\Lambda}_\epsilon$  and  $W^u \tilde{\Lambda}_\epsilon$  are  $\epsilon$ -close to the unperturbed ones.
- Using hypothesis **H2'**,  $W^s \tilde{\Lambda}_\epsilon \pitchfork W^u \tilde{\Lambda}_\epsilon$  along  $\Gamma_\epsilon$ .



- Combine the inner and the outer dynamics to construct a **transition chain** along  $\tilde{\Lambda}_\epsilon$ : sequence of whiskered tori with heteroclinic intersections, i.e.  $\{\mathcal{T}_i\}_{i=1}^N$ , such that  $\mathcal{W}^u(\mathcal{T}_i) \cap \mathcal{W}^s(\mathcal{T}_{i+1})$  and  $|I_N - I_1| = \mathcal{O}(1)$ .

- Use that

$$S_\epsilon(\tau_i) \cap_{\tilde{\Lambda}_\epsilon} \tau_{i+1} \Rightarrow W_{\tau_i}^u \cap W_{\tau_{i+1}}^s$$

(conditions **H2''**, **H3''** and **H3'''**)

- There is an orbit  $\tilde{x}(t)$  that **shadows** the transition chain.

**Part II:** Fast numerical algorithms for the computation of  
invariant tori in Hamiltonian systems  
(in collaboration with Rafael de la Llave and Yannick Sire)

# Computation of Invariant tori

- Invariant torus of dimension  $\ell =$  quasi-periodic solution with  $\ell$  independent frequencies (primary and secondary, maximal and whiskered).
- **Importance.** Together with their connections organize the long term behavior of the system (celestial mechanics, chemistry, ...)
- **Numerical computation.** Contributions of people in the Dynamical Systems group of Barcelona (de la Llave, Gómez, Haro, Jorba, Mondelo, Simó, Villanueva, ...).
- **Goal:** Develop numerical algorithms following the theoretical results of KAM Theorem without Action-Angle variables ([dILGJV05],[FLS08]) and implement them numerically.

[dILGJV05] R. de la Llave, A. González, A. Jorba and J. Villanueva. KAM theory without action-angle variables, *Nonlinearity*,18(2):855–895,2005.

[FLS08] E. Fontich, R. de la Llave and Y. Sire. Construction of invariant whiskered tori by a parametrization method. Part I: Maps and flows in finite dimensions. Preprint, 2008.

# The invariance equation

- Consider a map  $F$  **exact symplectic** defined on  $(U \subset \mathbb{R}^d) \times \mathbb{T}^d$ .
- Assume that  $\omega \in \mathbb{R}^\ell$  is fixed and **Diophantine**, i.e. for some  $\nu, \tau > 0$ ,

$$|\omega \cdot k - n|^{-1} \leq \nu |k|^\tau \quad \forall k \in \mathbb{Z}^\ell - \{0\}, \quad n \in \mathbb{Z}$$

- We seek for an embedding  $K : \mathbb{T}^\ell \rightarrow \mathbb{R}^d \times \mathbb{T}^d$  that satisfies the **invariance equation**

$$F \circ K - K \circ T_\omega = 0$$

where  $T_\omega(\theta) = \theta + \omega$ .

- The dynamics of  $F$  restricted on the invariant torus (range of  $K$ ) is conjugated to a rigid rotation of frequency  $\omega$ .
- Develop a **Newton method** to compute  $K$ .

## Some remarks on the algorithms

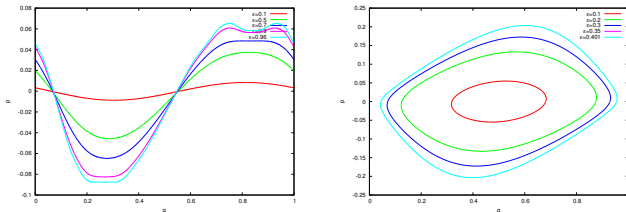
- Algorithms are efficient in the following sense: If we discretize  $K$  using  $N$  Fourier coefficients, the algorithm requires storage of  $\mathcal{O}(N)$  and the Newton step takes  $\mathcal{O}(N \log N)$  operations using FFT.
- The method does not require the system to be written in **Action-Angle variables** (it can deal in a unified way with both primary and secondary KAM tori).
- The system is not required to be close to the **integrable case**.

# KAM tori for the Standard Map

2D exact symplectic map defined on the cylinder  $\mathbb{R} \times \mathbb{T}$ .

$$\bar{p} = p + \varepsilon / (2\pi) \sin(2\pi q)$$

$$\bar{q} = q + \bar{p} \pmod{1}$$



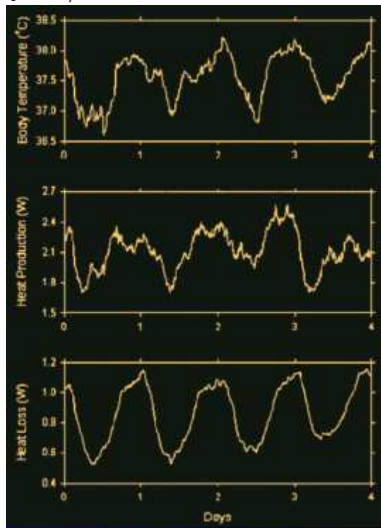
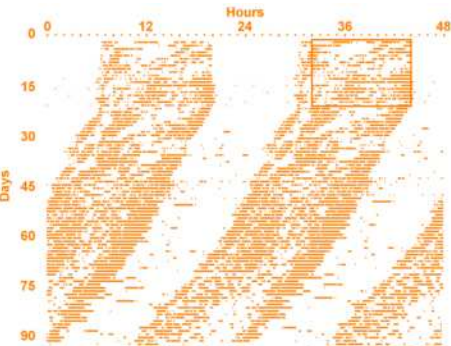
**Figure:** (Left) Primary tori of frequency  $\omega_g = (\sqrt{5} - 1)/2$  (golden mean) for values of  $\varepsilon = 0.1, 0.5, 0.7, 0.9, 0.96$ . They are shifted to have 0 offset. We used  $N = 2^{11}$  Fourier modes. It takes 0.03 sec to perform one step of the continuation method. (Right) Secondary tori of frequency  $3/40\omega_g$  for values of  $\varepsilon = 0.1, 0.2, 0.3, 0.35, 0.401$ . We used  $N = 2^9$  Fourier modes. It takes 0.01 sec to perform one step of the continuation method.



## Part III: A computational and geometric approach to Phase Resetting Curves and Surfaces

# Biological motivation: circadian rhythms

Biological clocks  $\approx$  Presence of limit cycles/oscillators



Consider an autonomous system

$$\dot{x} = X(x), \quad x \in \mathbb{R}^d, d \geq 2$$

with a periodic orbit  $\gamma$  of period  $T$

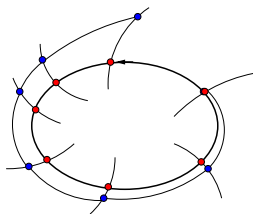
### Definition

A point  $q \in \Omega \subset \mathbb{R}^d$ ,  $\Omega$  open domain containing the limit cycle  $\gamma$ , is in **asymptotic phase** with a point  $p \in \gamma$  if

$$\lim_{t \rightarrow \infty} |\Phi_t(q) - \Phi_t(p)| = 0,$$

where  $\Phi_t$  is the flow associated to the vector field  $X$ .

The set of points having the same asymptotic phase is called **isochron**.  $\gamma$  is **isochronous** if every point in  $\Omega$  is in phase with a point on  $\gamma$ .



[Guck75] If  $\gamma$  is a **stable limit cycle**, then  $\gamma$  is **isochronous**. The isochrons are the leaves of the stable manifold  $W_{\gamma(\theta)}^s$ .

# Generalization of the phase in a neighborhood of the limit cycle

In a neighborhood  $\Omega$  of the limit cycle  $\gamma$  there exists a unique scalar function

$$\begin{aligned} \vartheta : \Omega \subset \mathbb{R}^d &\rightarrow \mathbb{T} = [0, 1) \\ x &\mapsto \vartheta(x) \end{aligned}$$

such that

$$\lim_{t \rightarrow \infty} |\Phi_t(x) - \gamma(\vartheta(x) + t/T)| = 0.$$

The value  $\vartheta(x)$  is the **asymptotic phase** of  $x$ . The **isochrons** are the **level sets** of the function  $\vartheta(x)$ .

# Phase Resetting Curves

Consider

$$\dot{x} = X(x) + \epsilon \delta(t(1 - \theta_s))$$

where  $\epsilon = (\epsilon_1, \dots, \epsilon_d)$ , then

$$PRC(\theta) = \theta_{new} - \theta.$$

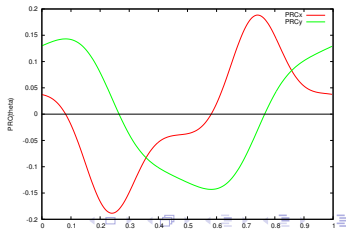
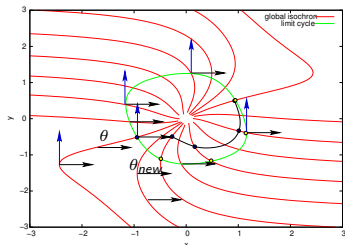
For weak perturbations,  
 $|\epsilon| \ll 1$ , the infinitesimal PRC

$$PRC(\vartheta(x)) = \epsilon \cdot \nabla \vartheta(x).$$

**PRC:**  $x \in \gamma$ .

**PRS:** Generalization for  $x \in \Omega$ .

Biological relevance of PRS



# Phase Resetting Curves

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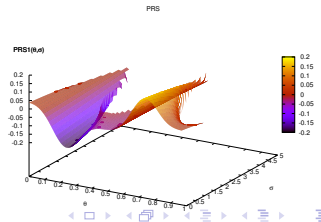
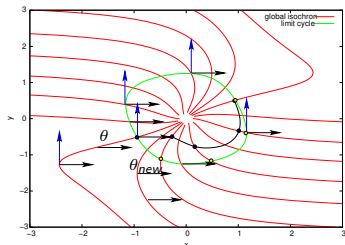
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**PRS:** Generalization for  $x \in \Omega$ .

Biological relevance of PRS



# Conclusions

- We proved the existence of **diffusing orbits** for a priori unstable Hamiltonian systems with a **generic** perturbation  $h$  assuming that it is regular enough.
- We developed **fast numerical algorithms** to compute invariant to tori (primary and secondary, maximal and hyperbolic).
- We **implemented** them and we applied them to compute primary and secondary maximal tori of the standard map and primary maximal and whiskered tori of the Froeshclé map.
- We extend the Phase Resetting Curves to a neighborhood of the limit cycle, obtaining what we call the **Phase Resetting Surface** and we computed them numerically.