Scattering maps for the hydrogen atom in a circularly polarized microwave field

Hamiltonian Dynamical Systems in Honor of Jean-Pierre Marco, Paris, June 7–10, 2021

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June 7th, 2021

Let us consider the relative motion of a hydrogen atom subjected to a circularly polarized (CP) microwave. In the simplest case (assuming planar motion for the electron) the *classical* motion is governed by a system of 2 2nd-order ODE

$$\ddot{X} = -\frac{X}{R^3} - F\cos(\omega s), \qquad R^2 = X^2 + Y^2,$$
$$\ddot{Y} = -\frac{Y}{R^3} - F\sin(\omega s), \qquad \dot{} = \frac{\mathrm{d}}{\mathrm{d}s},$$

where $\omega > 0$ is the *angular frequency of the microwave field* and $F > 0$ is the *field strength*.

This system can be written as a periodic in time 2 d.o.f Hamiltonian

$$H(X, Y, P_X, P_Y) = \frac{1}{2}\left(P_X^2 + P_Y^2\right) - \frac{1}{R} + F\left(X\cos\left(\omega s\right) + Y\sin\left(\omega s\right)\right).$$

As in the R3BP, one cat get rid of the time dependence introducing rotating coordinates (x, y, p_x, p_y) plus some scaling in time:

$$H = \frac{1}{2}(p_x^2 + p_y^2) - (xp_y - yp_x) - \frac{1}{r} + Kx, \qquad r = \sqrt{x^2 + y^2},$$

where $K = F/\omega^{4/3} > 0$, with associated Hamiltonian equations

$$\dot{x} = p_x + y, \qquad \dot{p}_x = p_y - \frac{x}{r^3} - K,$$

$$\dot{y} = p_y - x, \qquad \dot{p}_x = -p_x + \frac{y}{r^3},$$

invariant under the reversibility $(t, x, y, p_x, p_y) \to (-t, x, -y, -p_x, p_y)$.

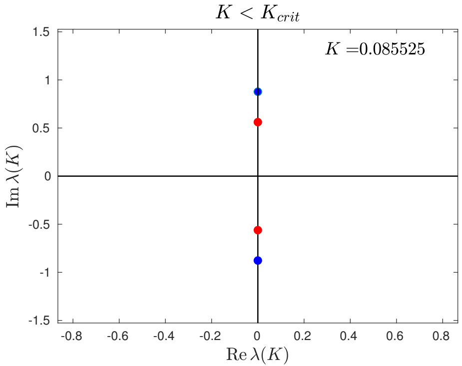
Remark: When $K = 0$ we obtain the rotating Kepler problem. We will be playing with the parameter K and the energy h, the value of the Hamiltonian H.

L_1 and L_2 (located on the x axis, their location varies with K)

- L_1 is a center$\times$saddle for all K, with characteristic exponents

$$\pm \mathrm{i}\sqrt{1+K}(1+\mathcal{O}(K)), \quad \pm\sqrt{3K}(1+\mathcal{O}(K)).$$

  - 1-d invariant manifolds, $W^u(L_1)$, $W^s(L_1)$ for $h = h(L_1) = h_1$
  - saddle Lyapunov periodic orbits $OPL_1(h)$ around L_1 for $h > h_1$



L_2 is a center$\times$center for $K < K_{crit} = \dfrac{1}{6\sqrt[3]{3}} = 0.11556\ldots$:

- elliptic PO
- 2-d tori

- Equilibrium points $L_1, \ldots, L_5$; $L_{1,2,3}$ are center$\times$saddle. $L_{4,5}$ have a transition from center$\times$center to a complex saddle for the mass parameter μ_R. Also a Hopf bifurcation.
- There are two singularities on the equations (collisions with the primaries), for the R3BP $\longleftrightarrow$ Just collision at the origin (for the CP problem).

So:

$$L_1 \text{ for the CP problem} \longleftrightarrow L_3 \text{ for the R3BP}$$
$$L_2 \text{ for the CP problem} \longleftrightarrow L_{4,5} \text{ for the R3BP}$$

- For $h_1 < h < h_1^*$ there exists a (saddle) Lyapunov orbit $OPL_1(h)$.
- $\Lambda = \bigcup_{h_1<h<h_1^*} OPL_1(h)$ is a NHIM (normally hyperbolic invariant manifold).
- Any Lyapunov orbit $OPL_1(h)$ possesses 2D whiskers $W^{\mathrm{s,u}}OPL_1(h)$.
- Any trajectory $\gamma(h)$ contained in $W^{\mathrm{s}}OPL_1(h) \cap W^{\mathrm{u}}OPL_1(h)$ is a *homoclinic orbit* to $OPL_1(h)$.
- If $W^{\mathrm{s}}OPL_1(h)$, $W^{\mathrm{u}}OPL_1(h)$ intersect transversally on $\gamma(h)$ for some h, $\gamma(h)$ is called a *transverse homoclinic orbit*. The same happens for nearby h.
- For every $Z \in \gamma(h)$ there exist unique X_-, X_+ in $OPL_1(h)$ such that $\Phi(t, Z) - \Phi(t, X_\pm) \to 0$ as $t \to \pm\infty$, where $\Phi(t, Z)$ denotes the flow of the Hamiltonian system.
- Notice that if $Z' := \Phi(\tau, Z)$, $X'_\pm := \Phi(\tau, X_\pm)$, then $\Phi(t, Z') - \Phi(t, X'_\pm) \to 0$ as $t \to \pm\infty$.

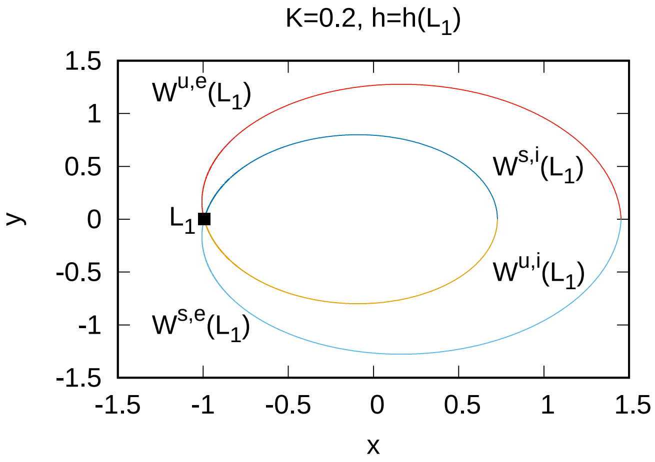
- For any transverse $\gamma(h)$, the associated scattering map is simply $X_- \in OPL_1(h) \mapsto X_+ \in OPL_1(h)$.
- In an adequate parameterization $X = X(\theta)$ such that $\dot\theta = 1$, the scattering maps is simply a translation $\theta \mapsto \theta + \Delta(h)$ by a phase shift $\Delta(h)$.
- Such scattering maps are also defined on the corresponding NHIM $\Lambda = \bigcup_{h_1<h<h_1^*} OPL_1(h)$ and take the simple form $(\theta, h) \mapsto (\theta + \Delta(h), h)$ of an *integrable twist map*, with a “real twist” as long as $\Delta'(h) \neq 0$.

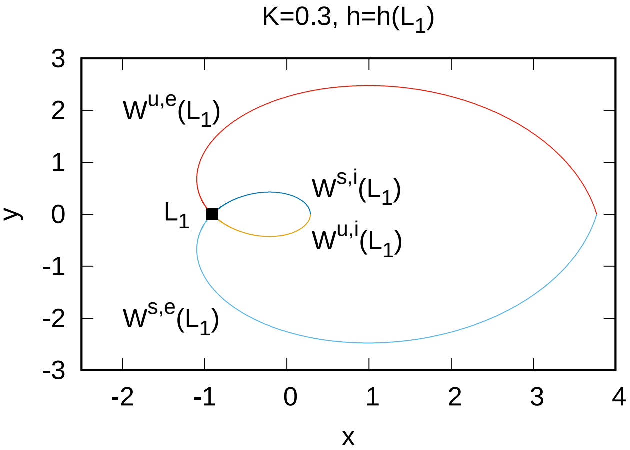
- Analytical/numerical analysis: For $K > 0$ small, the real characteristic exponent $\sqrt{3K}(1 + \mathcal{O}(K))$ is small, which makes difficult the computation of the invariant manifolds $W^{\mathrm{s,u}}OPL_1(h)$ associated to the Lyapunov orbits $OPL_1(h)$ and even more difficult the computation of their intersection (homoclinic orbits), since the splitting angle is exponentially small in K.
- 2D. And 3D?

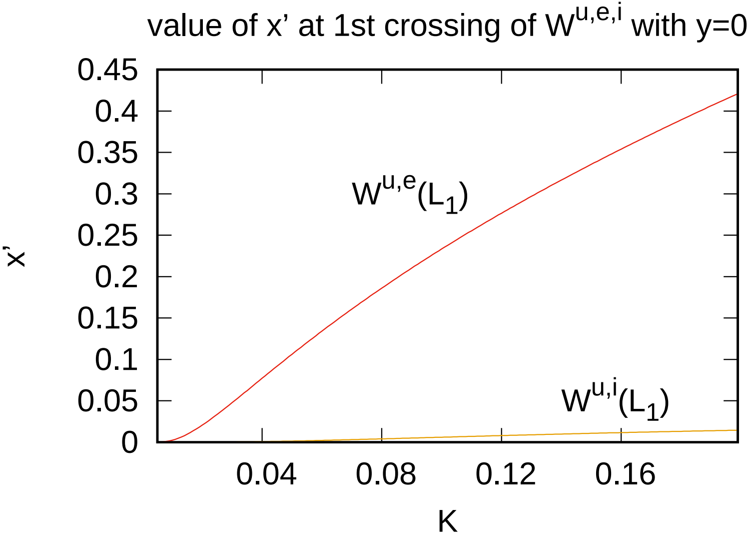
Theorem (Main result)

For $h_1^\star < h < h_1^*$, Each Lyapunov orbit $OPL_1(h)$ has exactly two transverse primary homoclinic orbits, giving rise to two different scattering maps defined on the NHIM, which are integrable twist maps.

Remark: by primary homoclinic orbits we mean that we consider just the *first* intersection of the invariant manifolds with the cross section $y = 0$.


K=0.2, h=h(L1)
1.5
1
0.5
0
-0.5
-1
-1.5
y
-1.5
-1
-0.5
0
0.5
1
1.5
x
Wu,e(L1)
Ws,i(L1)
L1
Wu,i(L1)
Ws,e(L1)


K=0.3, h=h(L1)
W^{u,e}(L1)
W^{s,i}(L1)
L1
W^{u,i}(L1)
W^{s,e}(L1)
3
2
1
0
-1
-2
-3
y
-2
-1
0
1
2
3
4
x


value of x' at 1st crossing of W^{u,e,i} with y=0
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
x'
0.04
0.08
0.12
0.16
K
W^{u,e}(L_1)
W^{u,i}(L_1)

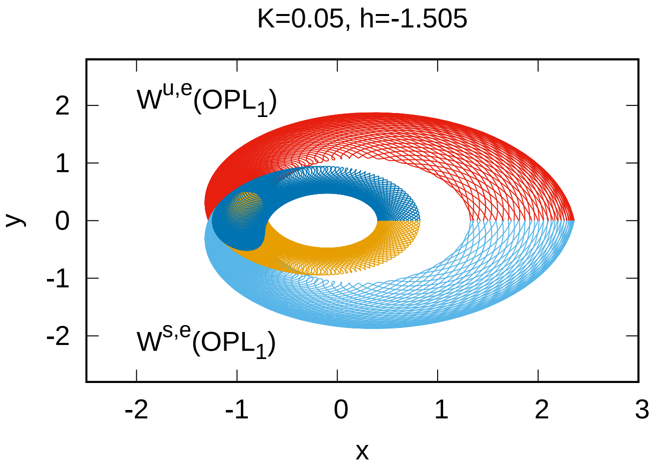


Figure: $W^{u,i}OPL_1(h)$ in orange and $W^{s,i}OPL_1(h)$ in dark blue.

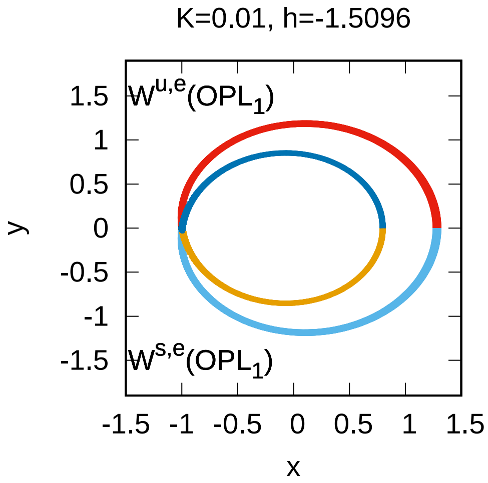


Figure: $W^{u,i} OPL_1(h)$ in orange and $W^{s,i} OPL_1(h)$ in dark blue.

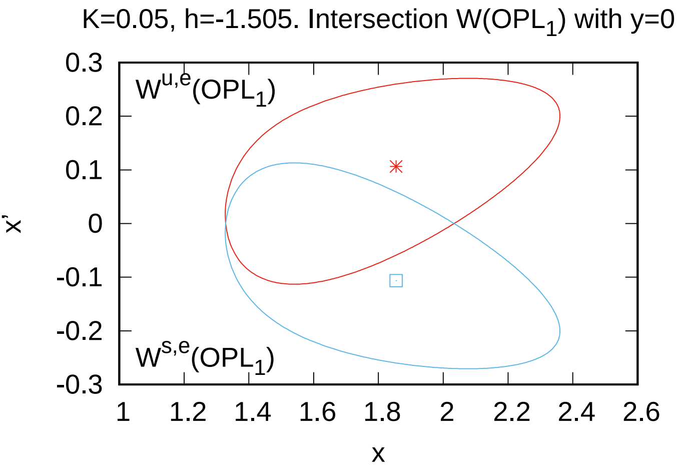


Figure: the orange asterisk is $W^{u,e}(L_1)$ and the dark blue square is $W^{s,e}(L_1)$.

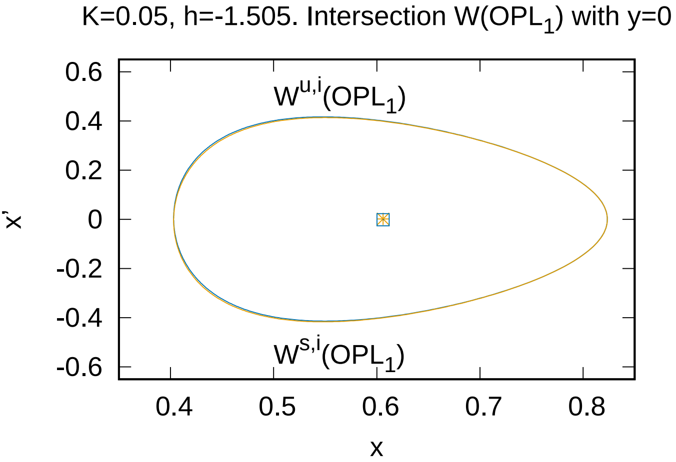


Figure: the orange asterisk is $W^{u,i}(L_1)$ and the dark blue square is $W^{s,i}(L_1)$.

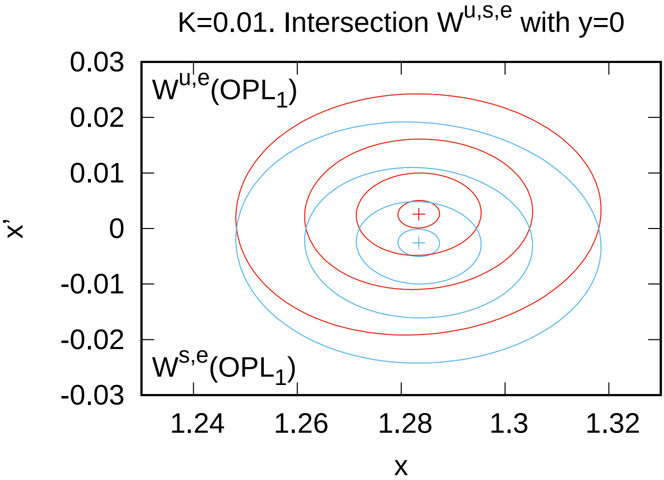


Figure: $W^{\mathrm{u,s,e}} OPL_1(h)$ for four different values of h and $K = 0.01$

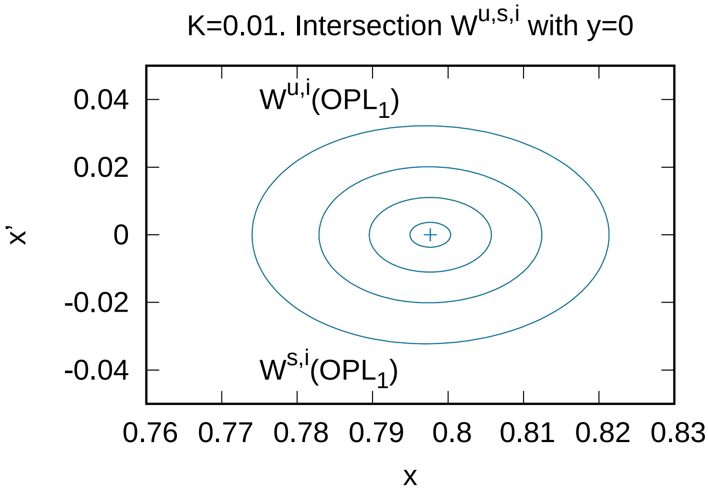


Figure: $W^{\mathrm{u,s,i}}OPL_1(h)$ for four different values of h and $K=0.01$

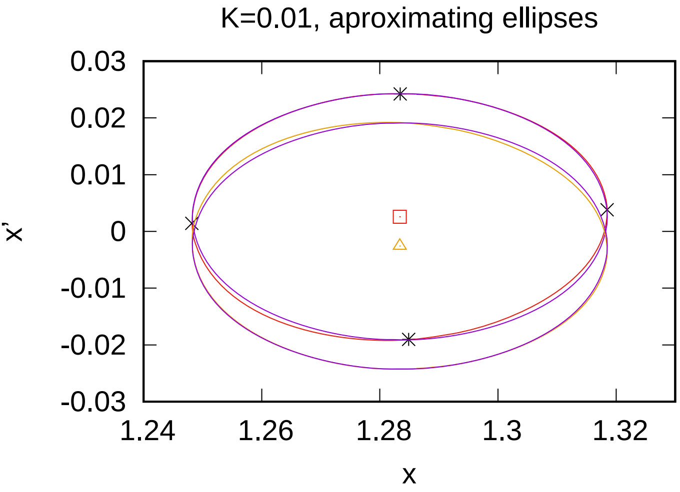


Figure: For small K, approximation of $W^{\mathrm{u,s,e}}OPL_1(h)$ by ellipses

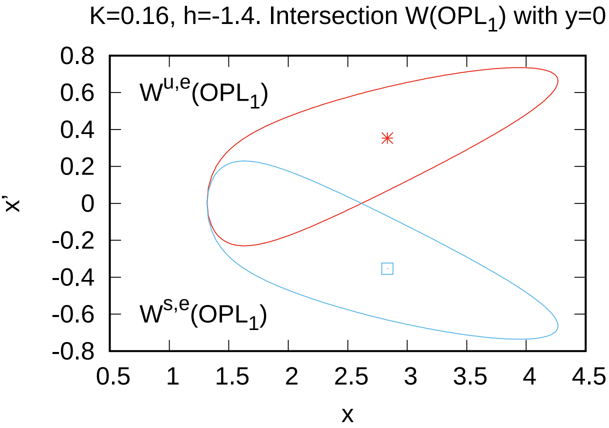


Figure: First cuts of $C^{\mathrm{u,s,e}}(h) := W^{\mathrm{u,s,e}} OPL_1(h) \cap \{y = 0\}$ in the variables (x, x') for $K = 0.16$ and $h = -1.4$. The angles in radians between $C^{\mathrm{u,e}}(h)$ and $C^{\mathrm{s,e}}(h)$ are $2 \cdot 1.2694$ and $2 \cdot -0.036$.

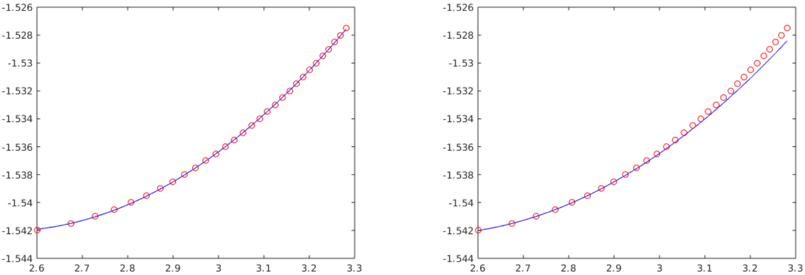
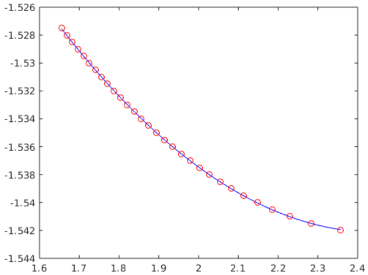


Figure: phase shift $\theta \mapsto \theta + \Delta(h)$ in the first external scattering map for $K = 0.16$ and $h = -1.4$ (with two different fits).



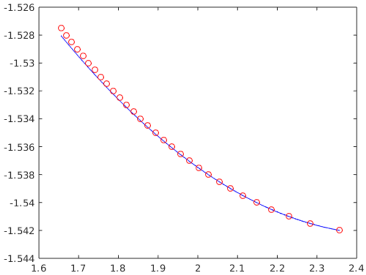


Figure: phase shift $\theta \mapsto \theta + \Delta(h)$ in the first external scattering map for $K = 0.16$ and $h = -1.4$ (with two different fits).

$$H = \frac{1}{2}(p_x^2 + p_y^2) - (xp_y - yp_x) - \frac{1}{r} + Kx, \qquad r = \sqrt{x^2 + y^2},$$

in *canonical polar coordinates* $(r, \theta, p_r, p_\theta)$ takes the form

$$H = \frac{1}{2}\left(p_r^2 + \frac{p_\theta^2}{2}\right) - p_\theta - \frac{1}{r} + Kr\cos\theta = H_{\mathrm{K}} - p_\theta + Kr\cos\theta.$$

In the *canonical Delaunay variables* (ℓ, g, L, G), which are the action-angle variables for the Kepler Hamiltonian H_{K} we have

$$H = -\frac{1}{2L^2} - G + K\left(L^2\cos E\cos g - LG\sin E\sin g - L^2 e\cos g\right),$$

where $e = \sqrt{1 - \frac{G^2}{L^2}}$ is the *eccentricity* and E is the *eccentric anomaly*: $\ell = E - e\sin E$.

The equilibrium point L_1 satisfies $L = G = 1$. Changing again and scaling

$$\ell = x + \pi + g, \quad g = -\varphi, L = 1 + \varepsilon^2 y, \quad G = 1 + \varepsilon^2 y - \varepsilon^2 I,$$

where $\varepsilon = \left(\frac{K}{3}\right)^{1/4}$ we get the singular a priori unstable Hamiltonian

$$H = \omega I + P(x, y) + \varepsilon h(\varphi, x, I, y; \varepsilon),$$

with $\omega = -\frac{1}{3\varepsilon^2}$ and

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

$$h(\varphi, x, I, y; \varepsilon) = \frac{3}{2}\sqrt{2I}\cos\varphi - \frac{1}{2}\sqrt{2I}\cos(2x + \varphi) + O(\varepsilon).$$

For $\varepsilon = 0$, the equilibrium point L_1 ($x = y = I = 0$) has the separatrices of the pendulum

$$x_0(t) = 4\arctan\left(\mathrm{e}^{\pm t}\right), \quad y_0(t) = \dot{x}_0(t) = \pm\frac{2}{\cosh t}.$$

The *Melnikov potential* associated to a periodic orbit $x = y = 0$ with action I is

$$\begin{aligned}\mathcal{L}(\theta, I) &= -\int_{\infty}^{\infty} \left(h(\theta + \omega\sigma, x_0(\sigma), I, y_0(\sigma); 0) - h(\theta + \omega\sigma, 0, I, 0; 0)\right) \mathrm{d}\sigma \\ &= \frac{8\pi}{3}\sqrt{2I}\,\omega^3\left(1 - \frac{2}{\omega^3}\right)\frac{\mathrm{e}^{c\pi\omega/2}}{1 - \mathrm{e}^{2\pi\omega}}\cos\theta,\end{aligned}$$

where $c = \begin{cases} 1 \text{ for } y_0(t) > 0 \text{ (external)} \\ 3 \text{ for } y_0(t) < 0 \text{ (internal)} \end{cases}$, $\omega = -\frac{1}{3\varepsilon^2}$.

- The analytical computations for the splitting of the separatrices of the Lyapunov orbits provided by the Poincaré-Melnikov method (more or less) agree with the numerical computations.
- Analogously for the splitting of the separatrices of L_1.
- Since the order ℓ of the singularity of the perturbation $\tau \mapsto h(\varphi, x_0(\tau), I, y_0(\tau); \varepsilon)$ (D-Seara97) is 4, greater than $r = 2$, the order of the singularity of the unperturbed Hamiltonian $P(x, y)$, we expect (Baldomá06) that the Melnikov potential will give the dominant part of the splitting.
- There is still no complete proof.
- The more interesting case is the spatial CP problem, where Arnold diffusion takes place.

Bon anniversaire, Jean-Pierre!!

Happy birthday, Jean-Pierre!!

Per molt anys, Jean-Pierre!!