Insight; not just numbers

Numerical continuation of solutions in conservative systems

Jorge Galán Vioque

Departamento de Matemática Aplicada &
Instituto de Matemáticas de la Universidad de Sevilla (IMUS)

with E. Freire (Sevilla), F. J. Muñoz-Almaraz (Cardenal Herrera, Valencia),
E. Doedel (Concordia, Montreal) and A. Vanderbauwhede (Ghent),
A. Bengochea and E. Pérez-Chavela (UAM).

Ddays

Ddays 2014
Badajoz, 13th November 2014

Insight?

Insight?

INSIGHT: Visión interna, percepción, (Gestalt) comprensión.

Insight?

INSIGHT: Visión interna, percepción, (Gestalt) comprensión.
STRUCTURAL INSIGHT = conocimiento consciente o inconsciente del sujeto que adquiere, emplea y proyecta **por medio de la unión de estructuras**

Insight?

INSIGHT: Visión interna, percepción, (Gestalt) comprensión.
STRUCTURAL INSIGHT = conocimiento consciente o inconsciente del sujeto que adquiere, emplea y proyecta **por medio de la unión de estructuras**

Computational Tools DS Group Sevilla

- Normal Forms.
- Numerical Continuation of solutions with AUTO.
- Symbolic and numerical Computations for PWLS.

Insight?

INSIGHT: Visión interna, percepción, (Gestalt) comprensión.
STRUCTURAL INSIGHT = conocimiento consciente o inconsciente del sujeto que adquiere, emplea y proyecta **por medio de la unión de estructuras**

Computational Tools DS Group Sevilla

- Normal Forms.
- Numerical Continuation of solutions with AUTO.
- Symbolic and numerical Computations for PWLS.
- Hamiltonian systems (JGV)

Insight?

INSIGHT: Visión interna, percepción, (Gestalt) comprensión.
STRUCTURAL INSIGHT = conocimiento consciente o inconsciente del sujeto que adquiere, emplea y proyecta **por medio de la unión de estructuras**

Computational Tools DS Group Sevilla

- Normal Forms.
- Numerical Continuation of solutions with AUTO.
- Symbolic and numerical Computations for PWLS.
- Hamiltonian systems (JGV)
- Numerical Methods for PDEs (BGA, RTNS2015)

Continuation of periodic orbits in Hamiltonian systems

Continuation of periodic orbits in Hamiltonian systems

What is the best computational approach?

What is the best computational approach?

Skilled programmer and/or long term project

UNIVERSIDAD DE SEVILLA

What is the best computational approach?

Skilled programmer and/or long term project

Be a man and write your own code!

or

What is the best computational approach?

Skilled programmer and/or long term project

Be a man and write your own code!

or

The wimpy approach

What is the best computational approach?

Skilled programmer and/or long term project

Be a man and write your own code!

or

The wimpy approach

Use a (good) black box code, but

What is the best computational approach?

Skilled programmer and/or long term project

Be a man and write your own code!

or

The wimpy approach

Use a (good) black box code, but
understand what you are doing and be careful.
In our case AUTO.

References

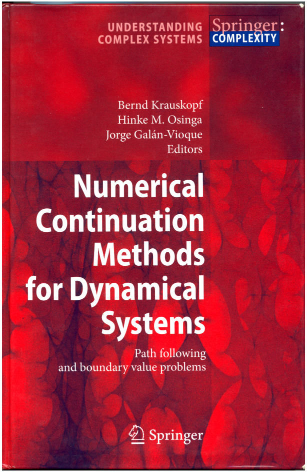
- Crash Course on Numerical Continuation:
  see article by E. Doedel in Scholarpedia

References

- Crash Course on Numerical Continuation:
  see article by E. Doedel in Scholarpedia
- Crash Course on using AUTO:
  The 4.5 minutes guide to AUTO *by F. Schilder.*

References

- Crash Course on Numerical Continuation:
  see article by E. Doedel in Scholarpedia
- Crash Course on using AUTO:
  The 4.5 minutes guide to AUTO *by F. Schilder.*



One idea and three examples

$$\dot{x} = f(x, \lambda)$$

One idea and three examples

$$\dot{x} = f(x, \lambda)$$

$$F(x, \lambda) = E$$

One idea and three examples

$$\dot{x} = f(x, \lambda)$$

$$F(x, \lambda) = E$$

1. How do we continue solution in the $\boxed{E}$ parameter?

One idea and three examples

$$\dot{x} = f(x, \lambda)$$

$$F(x, \lambda) = E$$

1. How do we continue solution in the $\boxed{E}$ parameter?
2. A simple example.

One idea and three examples

$$\dot{x} = f(x, \lambda)$$

$$F(x, \lambda) = E$$

1. How do we continue solution in the $\boxed{E}$ parameter?
2. A simple example.
3. Continuation in conservative systems or continuation without parameters; an alternative to reduction methods.

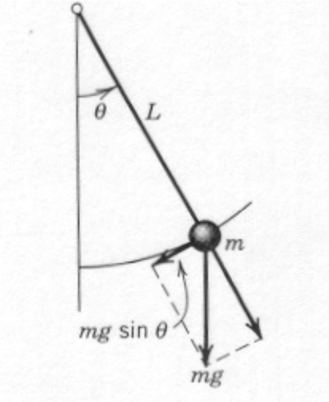
One idea and three examples

$$\dot{x} = f(x, \lambda)$$

$$F(x, \lambda) = E$$

1. How do we continue solution in the $\boxed{E}$ parameter?
2. A simple example.
3. Continuation in conservative systems or continuation without parameters; an alternative to reduction methods.
4. Three examples with insight.

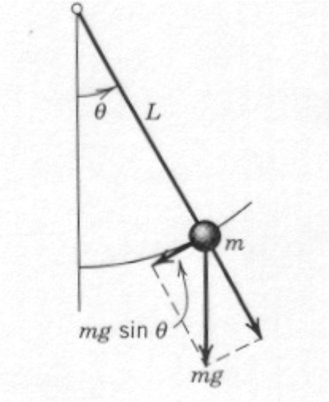
The best-seller in mathematical modelling



Galileo's pendulum

- 3 parameters: L, m, g

The best-seller in mathematical modelling



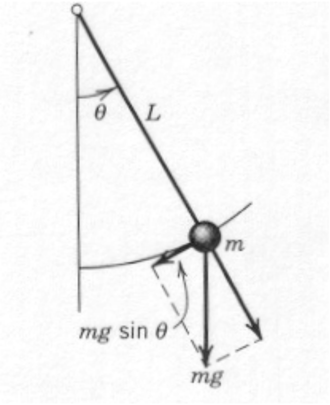
Galileo's pendulum

- 3 parameters: L, m, g
- Newton's second law:

$$mL\ddot{\theta} + mg\sin\theta = 0$$

-

The best-seller in mathematical modeling



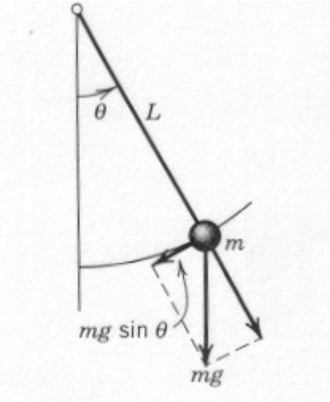
Galileo's pendulum

- 3 parameters: L, m, g
- Newton's second law:

$$\ddot{\theta} + \frac{g}{L}\sin\theta = 0$$

-

The best-seller in mathematical modeling



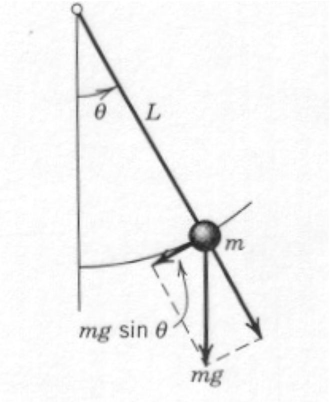
Galileo's pendulum

- Rescaling time with $\tau = \sqrt{\frac{L}{g}}$.
- Newton's second law:

Galileo's Pendulum Equation

$$\ddot{\theta} + \sin\theta = 0$$

The best-seller in mathematical modeling



Galileo's pendulum

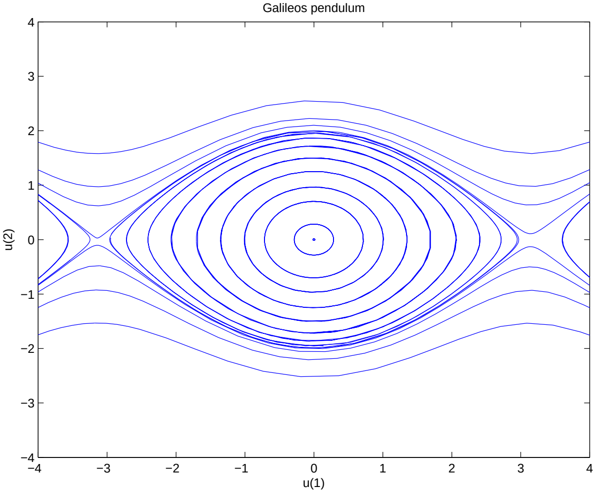
- Rescaling time with $\tau = \sqrt{\frac{L}{g}}$.
- Newton's second law:

Galileo's Pendulum Equation

$$\ddot{\theta} + \sin\theta = 0$$

- One dof ODE without parameters with two equilibria: $\theta = 0$ (S) and $\theta = \pi$ (U) and a one parameter family of periodic orbits.

Phase portrait of Galileo’s pendulum



The reduction method

- Position and velocity are not independent of each other.

The reduction method

- Position and velocity are not independent of each other.
- The system has a first integral or conserved quantity:

$$E = \frac{\dot{\theta}^2}{2} + 1 - \cos\theta.$$

The reduction method

- Position and velocity are not independent of each other.
- The system has a first integral or conserved quantity:

$$E = \frac{\dot{\theta}^2}{2} + 1 - \cos\theta.$$

- The dimension of the problem can be reduced by eliminating the velocity:

$$\dot{\theta} = \sqrt{2(E - 1 + cos\theta)}.$$

The reduction method

- Position and velocity are not independent of each other.
- The system has a first integral or conserved quantity:

$$E = \frac{\dot{\theta}^2}{2} + 1 - \cos\theta.$$

- The dimension of the problem can be reduced by eliminating the velocity:

$$\dot{\theta} = \sqrt{2(E - 1 + cos\theta)}.$$

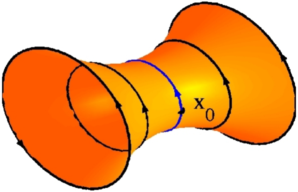
- We have introduced now *E* as an internal parameter that can be used for continuation (and lowered the dimension).

The general picture for Hamiltonian systems

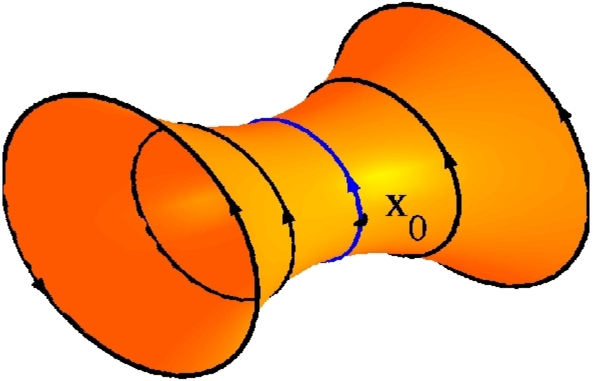
U open set in $\mathbb{R}^{2n}$, $H \in \mathcal{C}^1(U)$ con $J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$.

$$u' = J\nabla H(u)$$

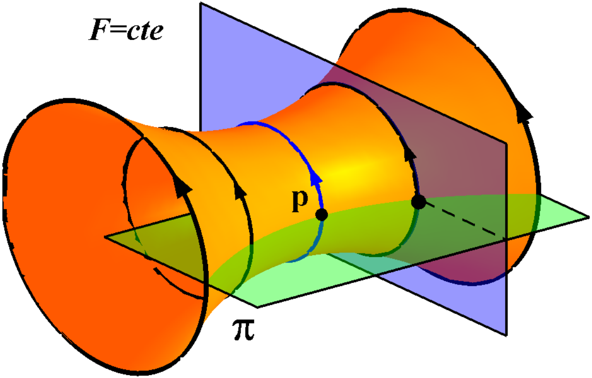
- ODE without explicit parameters.
- H is a conserved quantity.
- Periodic orbits are not isolated (cylinder theorem).



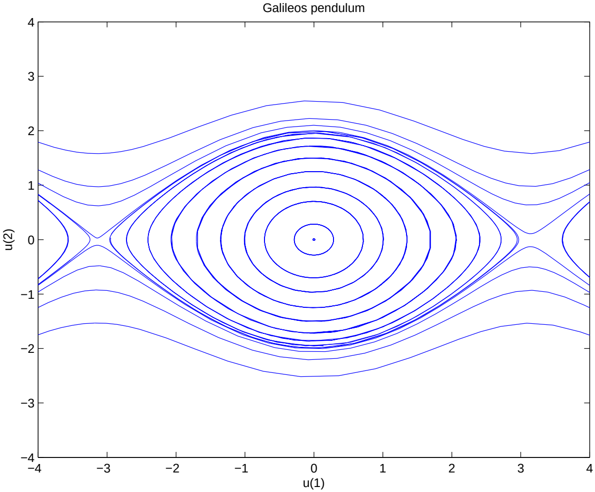
Geometrical picture: Cylinder Theorem



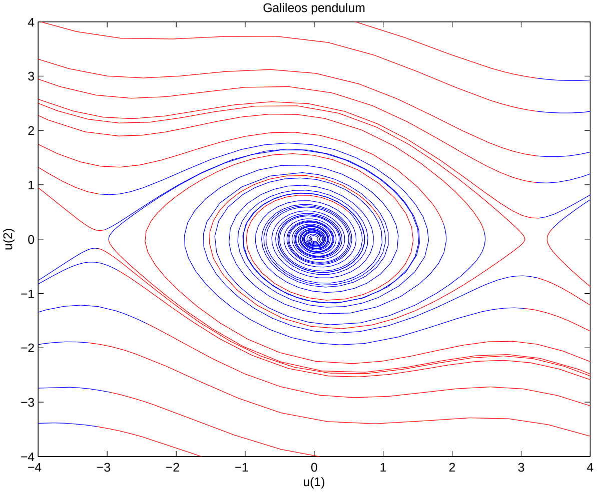
Geometrical picture: Reduction



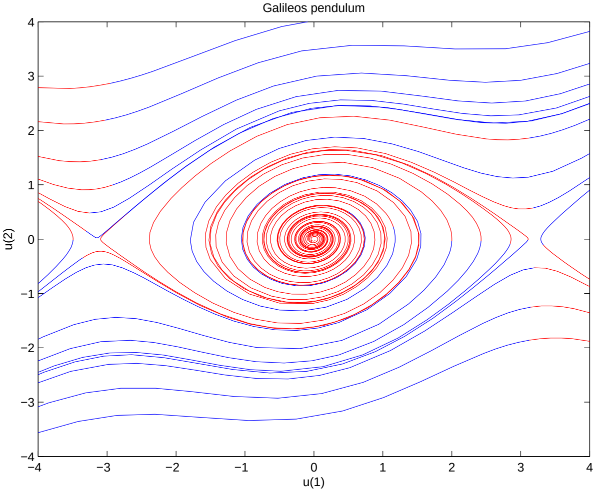
Alternative method: Increase the dimension!



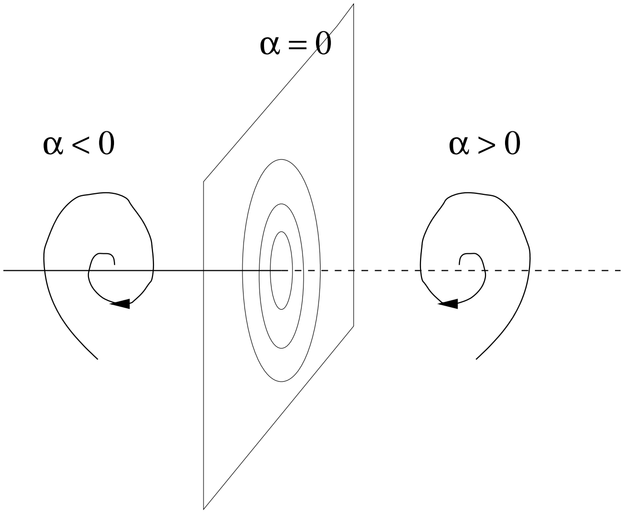
Alternative method: positive dissipation



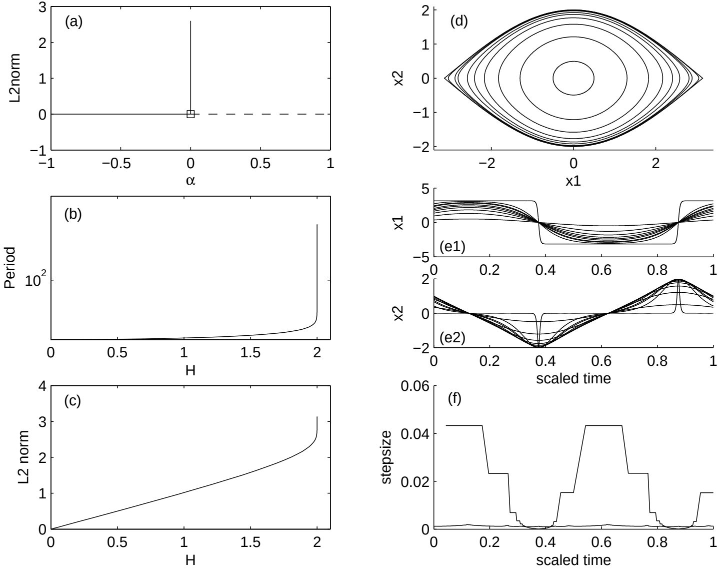
Alternative: negative dissipation



The idea: $\ddot{\theta} + \alpha\dot{\theta} + \sin\theta = 0$



AUTO results



Remarks

1. It is straightforward to implement
   (if we know the unfolding term) [Physica D **181** (2001)].
2. It can be extended to k independent conserved quatities.
3. Bifurcations can be detected and followed.
4. We can detect homo- and heteroclinic connections.
5. The computation preserves the simplectic character of the problem (Hamiltonian case).
6. For reversible system there are further simplifications.
7. AUTO is parallelized (Openmp and MPI)

Theory: BVP Formulation

$$u' = T(J\nabla H(u(t)) + \alpha \nabla H(u(t))), \qquad u(1) = u(0). \quad (1)$$

with u, α and T as unknowns. Finding a T-periodic orbit of $u' = J\nabla H(u)$ is equivalent to finding a solution of (1) if $\alpha = 0$. We have to include a phase condition to fix the time origin.

$$(u(0) - u_0(0))^* u_0'(0) = 0. \quad (2)$$

Continuation theorem with 1 conserved quantity

Theorem

Let $u_0(t)$ be a periodic solution with period $0 < T_0 < +\infty$ whose monodromy matrix has 1 as an eigenvalue with **geometric multiplicty one** or **algebraic multipicity two**. Then, there existis a unique branch of solutions of (1) and (2) in a neighbourhood of $(u, T, \alpha) = (u_0, T_0, 0)$. Moreover, along the branch $\alpha = 0$.

- The proof is a direct application of IFT and the fact that $H(u(t))$ is constant along the periodic orbit.

Generalization

- Let $\mathcal{W}_{\mathbf{p}} = \{\nabla F(\mathbf{p}) \,:\, F$ first ontegral of $\dot{x} = f(x)\}$, $\dim(\mathcal{W}_{\mathbf{p}}) = k$, $\varphi_t(\mathbf{x}, \boldsymbol{\alpha})$ the flow and $\mathrm{orb}_{\varphi}(\mathbf{p})$ the orbit.
- $\dot{x} = f(x) \quad \rightarrow \quad \dot{x} = f(x) + \alpha_1 \nabla F_1(x) + \ldots + \alpha_k \nabla F_k(x)$,

Proposition

Let $\mathbf{p} \in \mathbb{R}^n$ *s. t.* $\mathrm{orb}_{\varphi}(\mathbf{p})$ *be* $T-$*periodic. It holds that* $\mathrm{Im}(D\varphi_T(\mathbf{p}) - I) + \mathbb{R} f(\mathbf{p}) \subseteq \mathcal{W}_{\mathbf{p}}^{\perp}$.

General results

Definition (Normal periodic orbit)

Let $\mathbf{p} \in \mathbb{R}^n$ such that the orbit $\mathrm{orb}_\varphi(\mathbf{p})$ is periodic with period $T > 0$ and $\mathbf{p}$ is not an equilibrium of $\dot{\mathbf{z}} = f(\mathbf{z})$. We say that $\mathrm{orb}_\varphi(\mathbf{p})$ is a normal periodic orbit of e $\dot{\mathbf{z}} = f(\mathbf{z})$ if

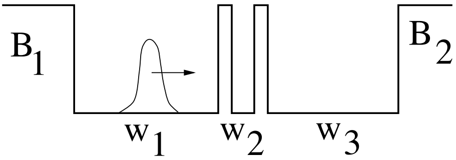
$$\mathrm{Im}(D\varphi_T(\mathbf{p}) - I) + \mathbb{R}f(\mathbf{p}) = \mathcal{W}_{\mathbf{p}}^{\perp}.$$

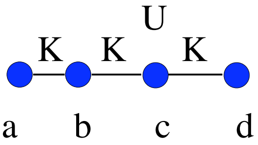
Theorem (Continuation with *k* conserevd quantities)

Let $\mathbf{p} \in \mathbb{R}^n$ *be a point that generates a* **normal** *periodic orbit of* $\dot{\mathbf{x}} = f(\mathbf{x})$ *with period* $T > 0$*. Then there exists a neighbourhood of* $T > 0$ *such that the set of points that generate periodic orbits whose period is in that neighbourhood of* T *is locally a submanifold at* $\mathbf{p}$*.*

Example 1: Chaos in a mean field quantum system

Jona-Lasinio et al[1], studied numerically the time-evolution of a wave packet in a triple quantum well with electrostatic interaction just in the narrow central well in the *mean field* approximation (*Hartree*) and found chaotic behavior.





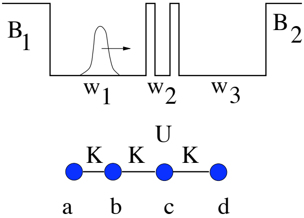
[1] G. Jona-Lasinio, C. Presilla and F. Capasso, Chaotic Quantum Phenomena without classical counterpart. Phys. Rev. Lett. **68** 2269 (1992)

Continuum model: localized NLSE

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + [V(x) + \alpha Q(t)\chi(x)]\Psi(x,t)$$

- $V(x)$ is the potential profile.
- $Q(t) = \int_{w_2} |\Psi(x,t)|^2 dx$ is the electronic charge in the central well (w_2).
- χ is a characteristic function which is one within well w_2 and zero elsewhere.
- α measures the electrostatic coupling.

Minimal discrete model



$$
\begin{aligned}
\dot{a} &= iKb \\
\dot{b} &= iKa + iKc \\
\dot{c} &= iKb + iKd - iU\bar{c}c^2 \\
\dot{d} &= iKc
\end{aligned}
$$

The wavefunction is $|\Psi >= |a\ b\ c\ d >\in \mathbb{C}^4$.

Classical Hamiltonian formulation

Reparameterizing time and the variables:

$$\begin{array}{rcl} \dot{a} & = & ib \\ \dot{b} & = & ia + ic \\ \dot{c} & = & ib + id - i\overline{c}c^2 \\ \dot{d} & = & ic \quad . \end{array}$$

$$\dot{z} = i\frac{\partial H(z,\overline{z})}{\partial \overline{z}}$$

$$H(z,\overline{z}) = \left(a\overline{b} + \overline{a}b + b\overline{c} + \overline{b}c + c\overline{d} + \overline{c}d\right) - \frac{(c\overline{c})^2}{2},$$

$z = (a, b, c, d)$. It is *autonomous*, *reversible* ($H(z,\overline{z}) = H(\overline{z}, z)$) and *invariant under diagonal rotations* in $\mathcal{C}^4$ ($z \to ze^{i\theta}$) $\to$ two conserved quantities.

Numerical evidence of chaotic behavior

Numerical integration: Fourier spectrum and Lyapunov exp.

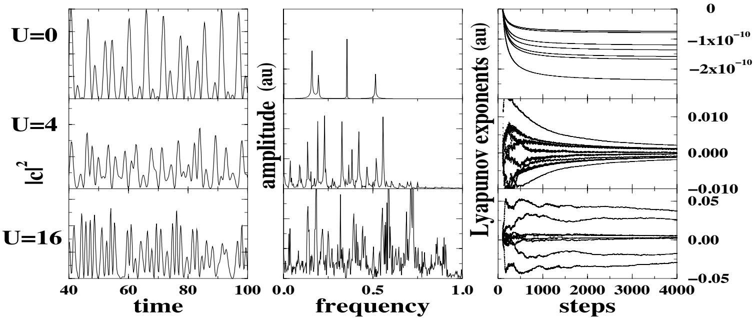


FIG. 2. Numerical results by simulation of (4), $K = 1$ and the same initial conditions. The upper row is the linear case ($U = 0$), the middle row is for $U = 4$ and the lower one for $U = 16$. The left column is the temporal evolution of the charge on the third site; $|c(t)|^2$. The central column is the Fourier spectrum of the signal and the right one shows the eight Lyapunov exponents. For $U = 0$ the system is quasiperiodic, whereas for $U = 4$ and $U = 16$ it is chaotic.

Insight: Origin of chaos and role of the Hartree states

- What is the origin of the chaotic behavior?
- What is the role of the Hartree solutions in the global picture?
  - Are they stable?
  - Are they the best solutions in the variational sense?
- Can we learn something new from the Hamitonian formulation?

Insight: Relative equilibria: Hartree selfconsistent states

In a rotating frame ($\omega \neq 0$)

$$z(t) = (a(t), b(t), c(t), d(t)) = e^{i\omega t}\,(A(t), B(t), C(t), D(t))\,,$$

$$\begin{aligned} \dot{A} &= i\,(B - \omega A) \\ \dot{B} &= i\,(A + C - \omega B) \\ \dot{C} &= i\,(B + D - \omega C) - i\,(C\overline{C})C \\ \dot{D} &= i\,(C - \omega D) \qquad . \end{aligned}$$

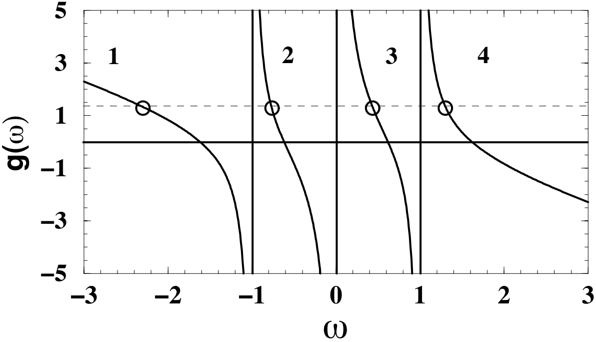
The equilibria correspond to *symmetric periodic orbits*.

$$A_0 = \frac{C_0}{\omega^2 - 1},\; B_0 = \frac{\omega}{\omega^2 - 1} C_0,\; D = \frac{C_0}{\omega},\; |C_0|^2 = -\frac{(\omega^2 - \phi^2)(\omega^2 - \frac{1}{\phi^2})}{\omega\,(\omega^2 - 1)}$$

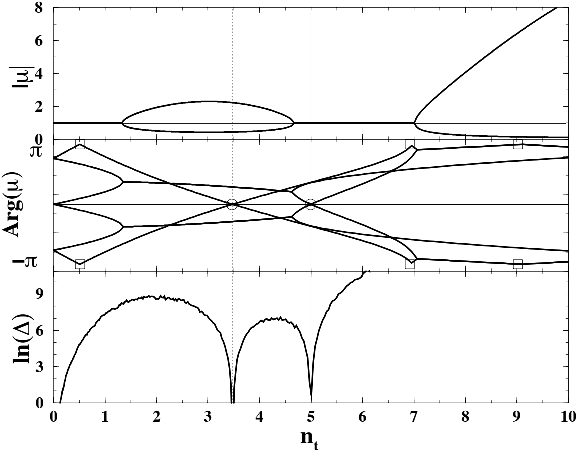
The four families of the Lyapunov center theorem

The sign of ω indicates the orientation of the orbit.

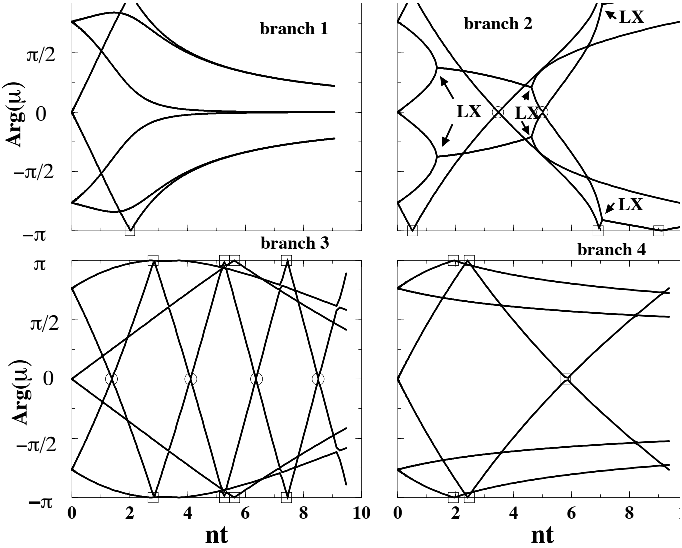
- $g(\omega) > 0 \rightarrow U > 0$ repulsive case.
- $g(\omega) < 0 \rightarrow U < 0$ attractive case.



Stability of the second branch: loxodromic bifurcations



Stability: the four branches



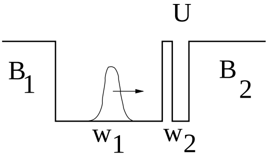
Can we lower the dimension?

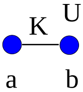
$$H(z,\bar{z}) = a\bar{b} + \bar{a}b - \frac{|b|^2}{2}$$

$$z = (a, b) \ \in \mathbb{C}^2.$$

- Reversible and symmetric $z \to e^{i\theta} z$.
- Two conserved quantities; H and $F = |z|^2$.
- Integrable

$$\begin{aligned} \dot{a} &= & & ib \\ \dot{b} &= & ia & -i\bar{b}b^2. \end{aligned}$$

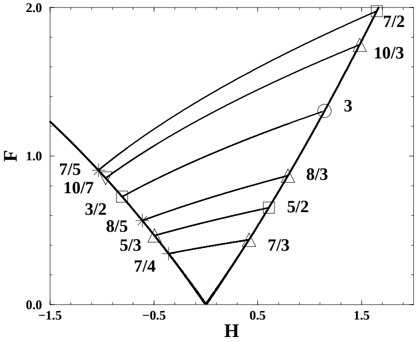


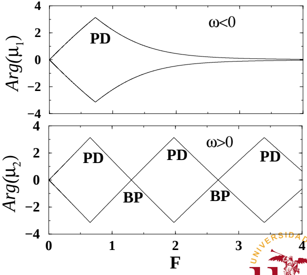


Relative equilibria and "bridges"

- $z = (0,0)$ unique equilibrium $\longrightarrow$ two Lyapunov families.
- In a rotating frame we can compute the Floquet multipliers

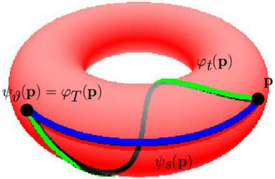
$$\mu_3 = \bar{\mu}_4 = e^{iT\sqrt{\omega^2+\frac{3}{\omega^2}}} = e^{i2\pi\sqrt{1+\frac{3}{\omega^4}}}$$





Rotation Number

- Let us consider the *flow induced by the symmetry* as the cross section (Σ).
- Choose an initial point $x \in \Sigma$ and let it flow.
- Look for the next intersection and measure the time T



$$\varphi^F_{2\pi\Theta}(x) = \varphi^H_T(x).$$

Global reduction

Following global reduction techniques [2] we can write the rotation number as

$$\Theta = \frac{1}{\pi}\int_{u_-}^{u_+} \frac{H + \frac{u^2}{2}}{2(F-u)} \frac{du}{\sqrt{Q(u)}}.$$

where

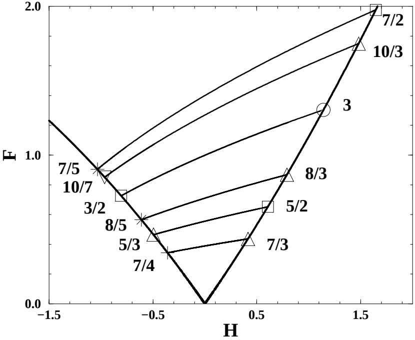
$$Q(u) = F^2 - \left(H + \frac{u^2}{2}\right)^2 - (F-2u)^2.$$

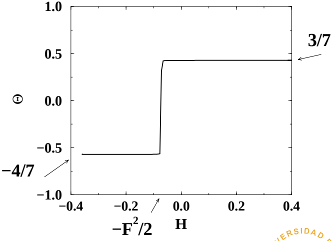
[2] R. Cushman & M. Bates, *Global aspects of classical integrable systems*. Birkhauser, 1997

The rotation number is constant along the bridge

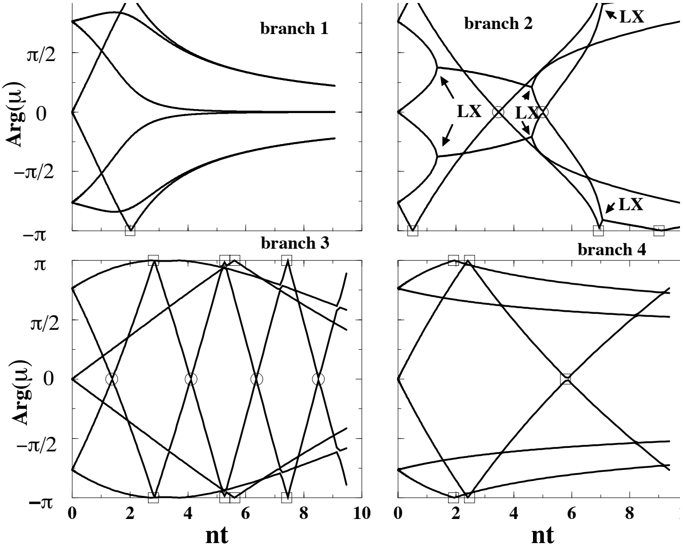
Theorem:

$$\frac{3}{7} = 1 - \frac{4}{7}$$

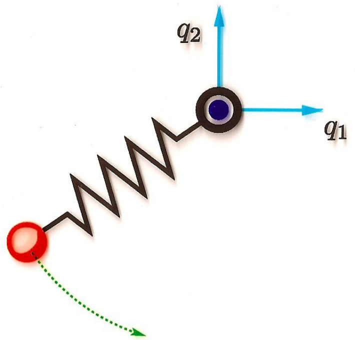




What are the bridges is this case?



Example 2: Elastic Pendulum

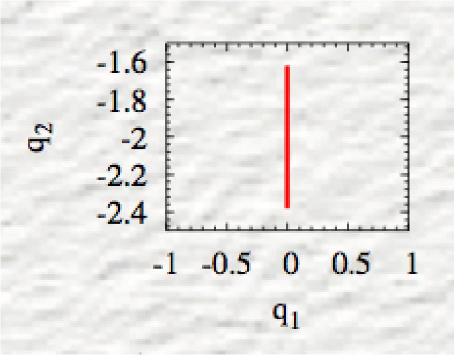


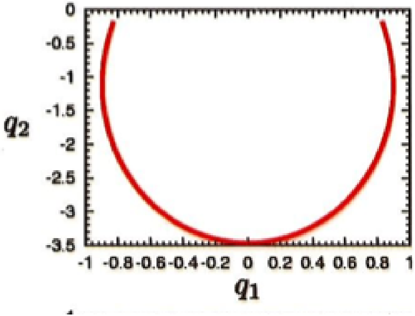
Adimensional parameter $\lambda = \frac{lk}{mg}$

Equilibria $\begin{cases} (0, -\lambda - 1) & \text{Stable} \\ (0, \lambda - 1) & \text{Unstable } (\lambda > 1) \end{cases}$

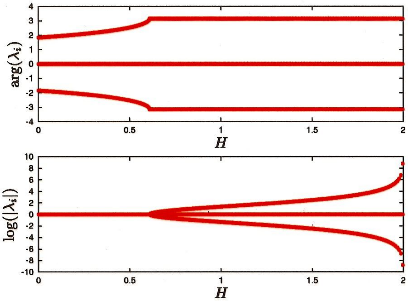
$$H = \frac{p_1^2}{2} + \frac{p_2^2}{2} + \frac{1}{2}\left(\sqrt{q_1^2 + q_2^2} - \lambda\right)^2 + q_2 + \lambda + \frac{1}{2}.$$

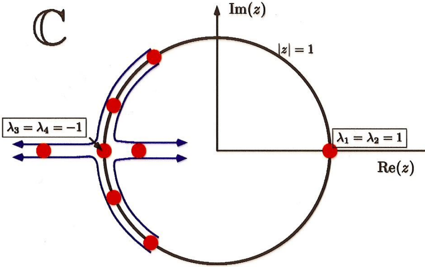
Reversibility continuation: Normal modes



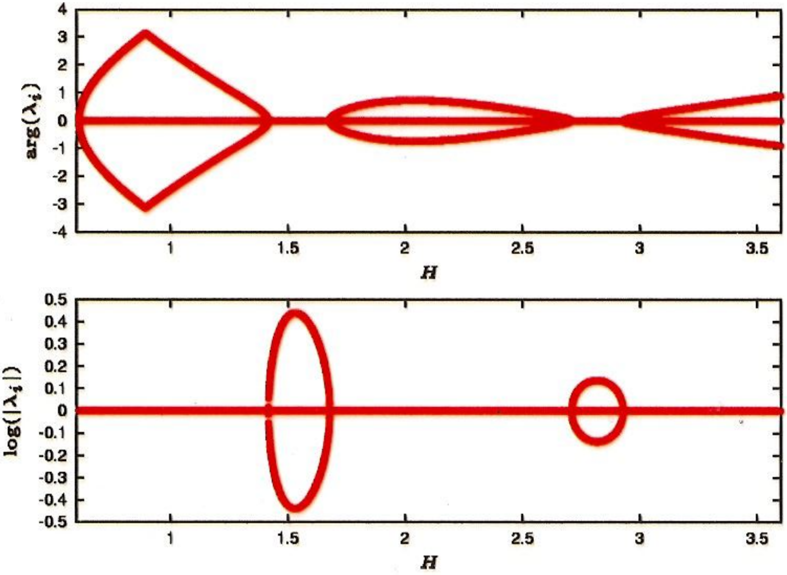


Vertical Nonlinear Normal Mode: Period Doubling

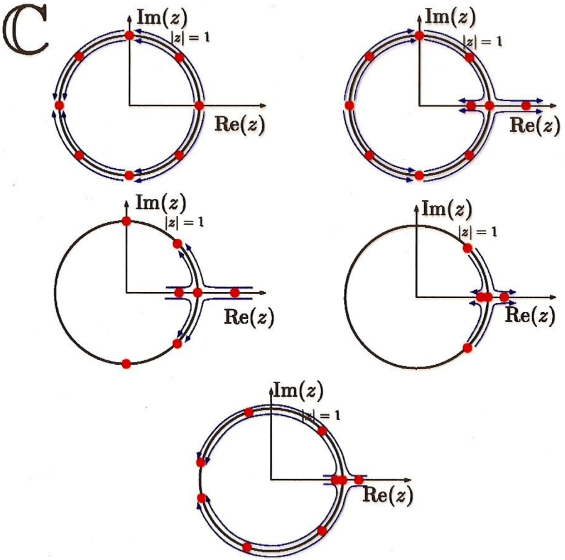




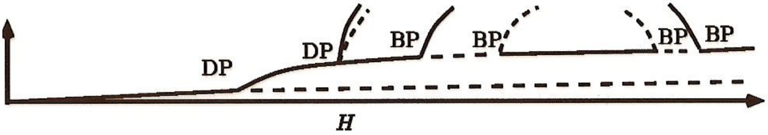
Period doubled branch



Period doubled branch



Schematic bifurcation diagram

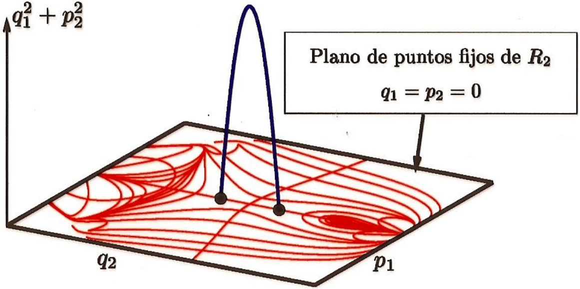


Reversibility continuation

Definition: We say that $R \in L(\mathbb{R}^n)$ is a reversibility for the system $\dot{\mathbf{x}} = f(\mathbf{x})$, if $Rf(\mathbf{x}) = -f(R\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^n$.

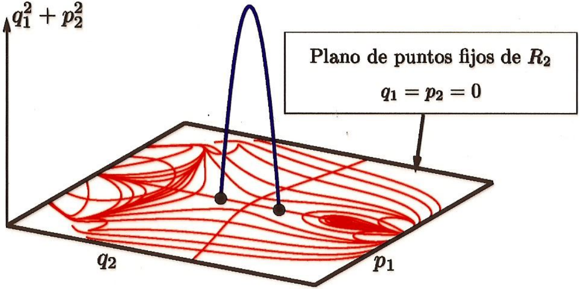
Reversibility continuation

Definition: We say that $R \in L(\mathbb{R}^n)$ is a reversibility for the system $\dot{\mathbf{x}} = f(\mathbf{x})$, if $Rf(\mathbf{x}) = -f(R\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^n$.



Reversibility continuation

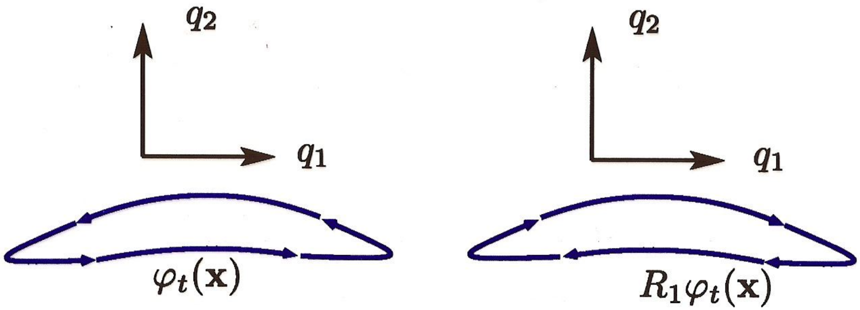
Definition: We say that $R \in L(\mathbb{R}^n)$ is a reversibility for the system $\dot{\mathbf{x}} = f(\mathbf{x})$, if $Rf(\mathbf{x}) = -f(R\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^n$.



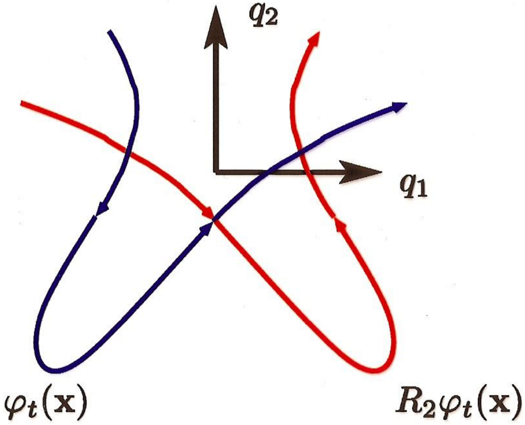
Example: in a mechanical system changing the sign to all velocities and integrate in negative time we get another solution.

Poetic definition: In an reversible system the **future** is the **past** of a

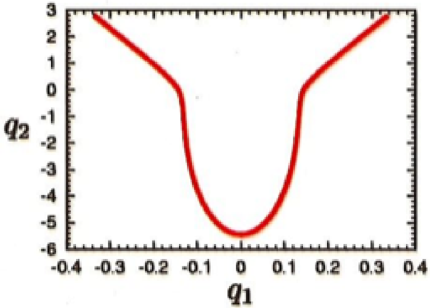
Reversibility continuation: R1

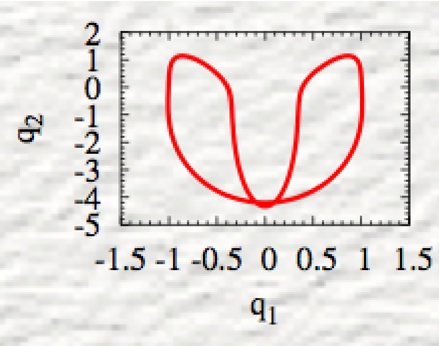


Reversibility continuation: R2

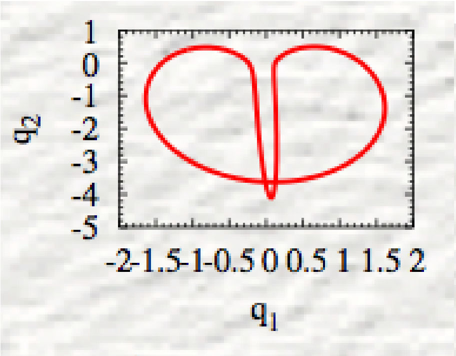


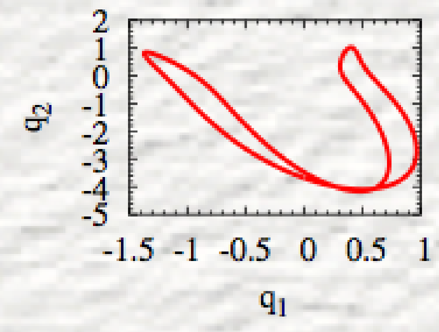
Reversibility continuation: reversible orbits



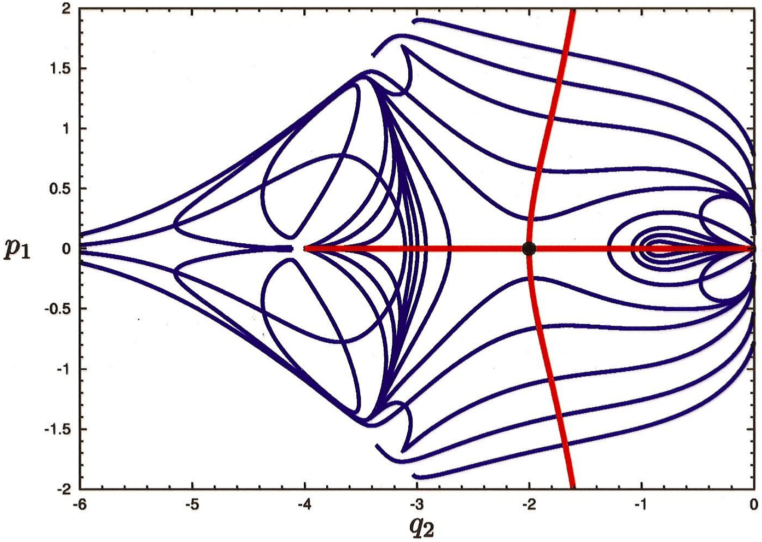


Reversibility continuation: non reversible orbits

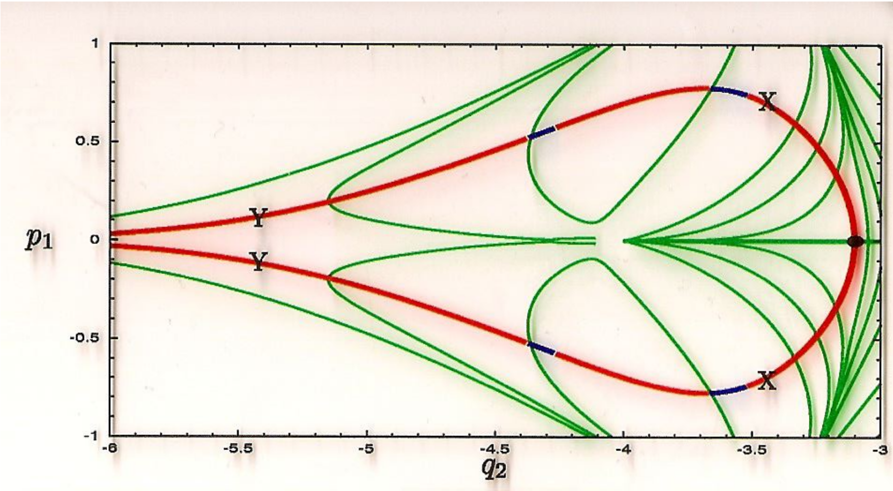




Insight: Reversibility continuation results

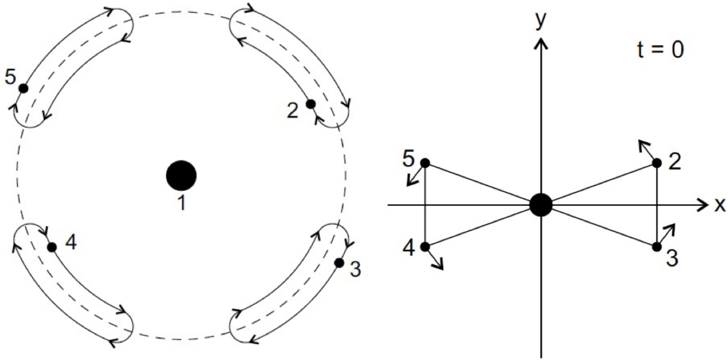


Insight: Reversibility continuation results



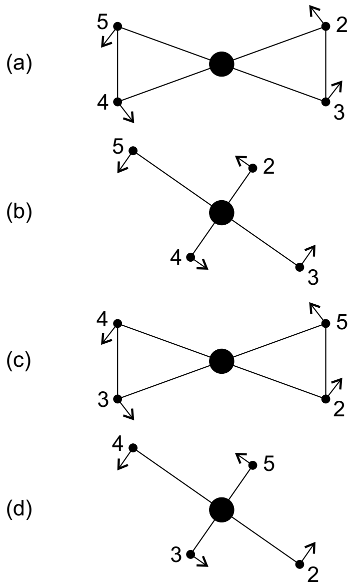
Horseshoe (exchange) solution of the 2k+1 BP

Not enough insight yet

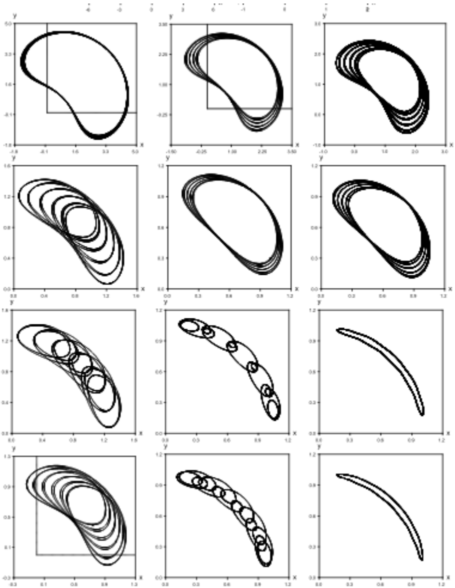


No overtaking condition

5 body exchange orbit



5 body exchange orbits



5 body exchange orbit connected to Euler-like solution