Transport in Hamiltonian Systems With Two or More Degrees of Freedom

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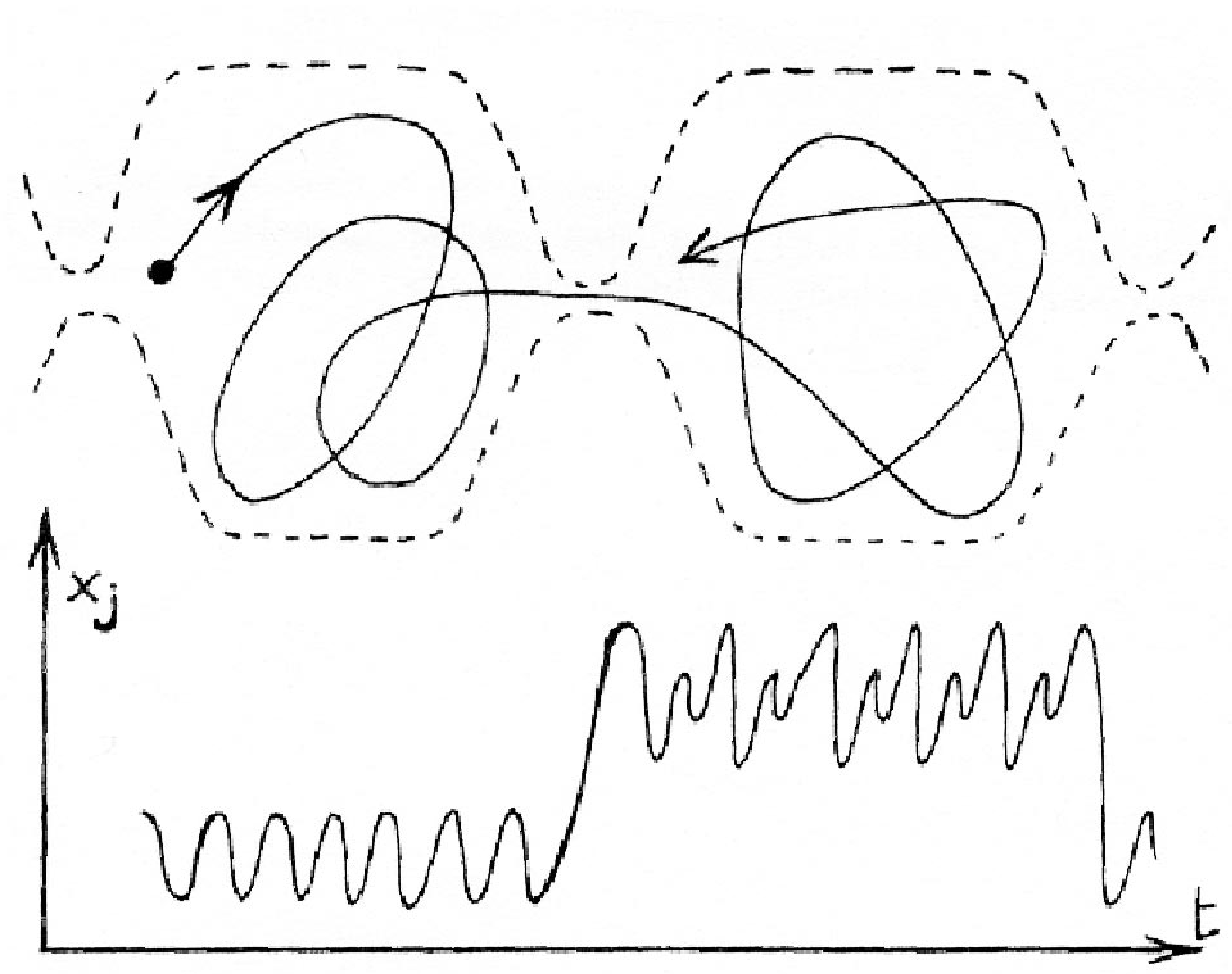
Outline

- ***Transport theory***
  - Time-independent Hamiltonian systems
  - with 2 degrees of freedom
  - with 3 (or N) degrees of freedom
    - **Example: restricted three-body problem**

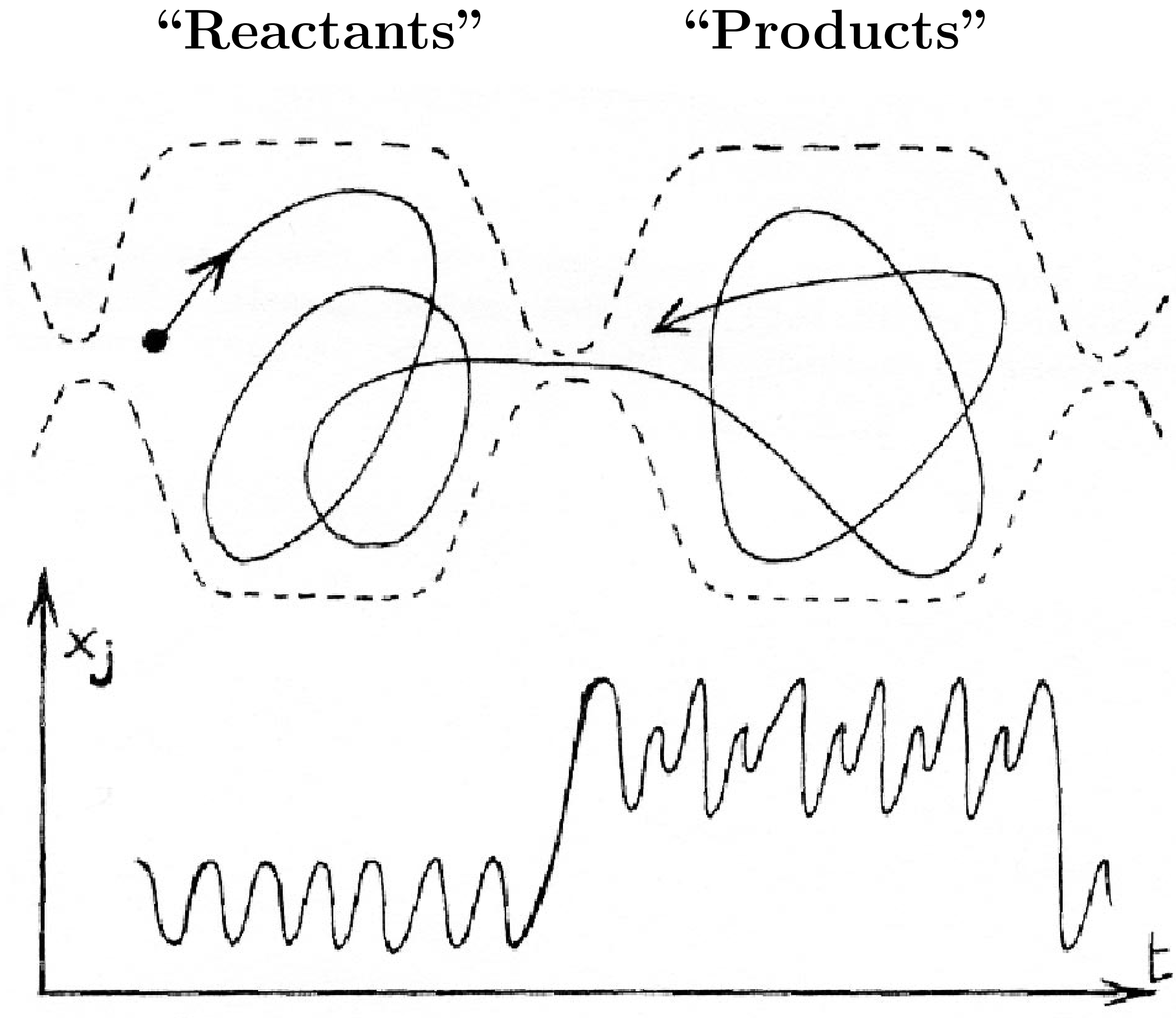
Chaotic Dynamics



Transport Theory

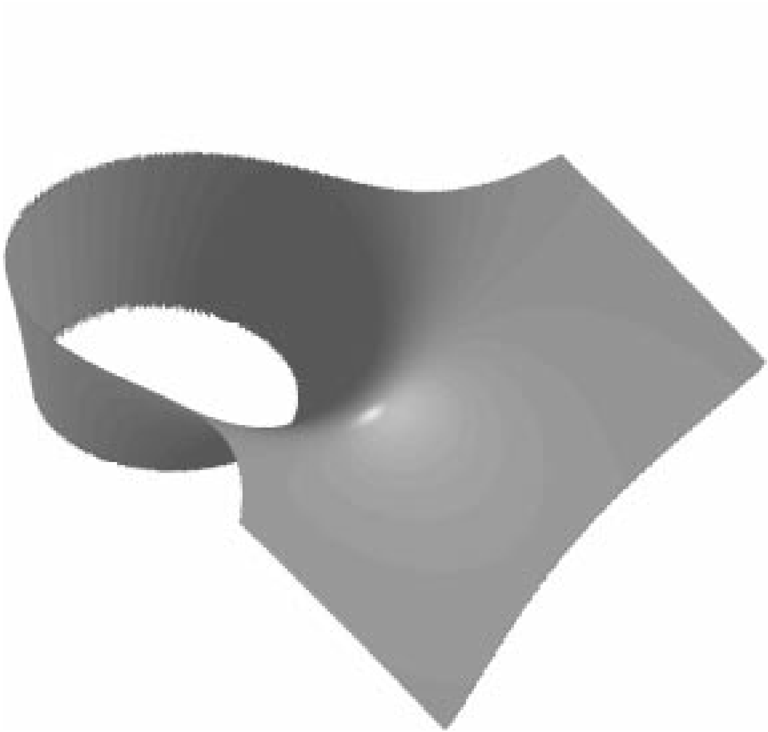
- ***Chaotic dynamics***
  → statistical methods
- ***Transport theory***
  - Motion of ensembles of trajectories in phase space
  - Asks: How long to move from one region to another?
  - Determine transition probabilities, correlation functions
  - Applications:
    - **Atomic ionization rates**
    - **Chemical reaction rates**
    - **Comet transition rates**
    - **Asteroid collision probabilities**

Partition the Phase Space

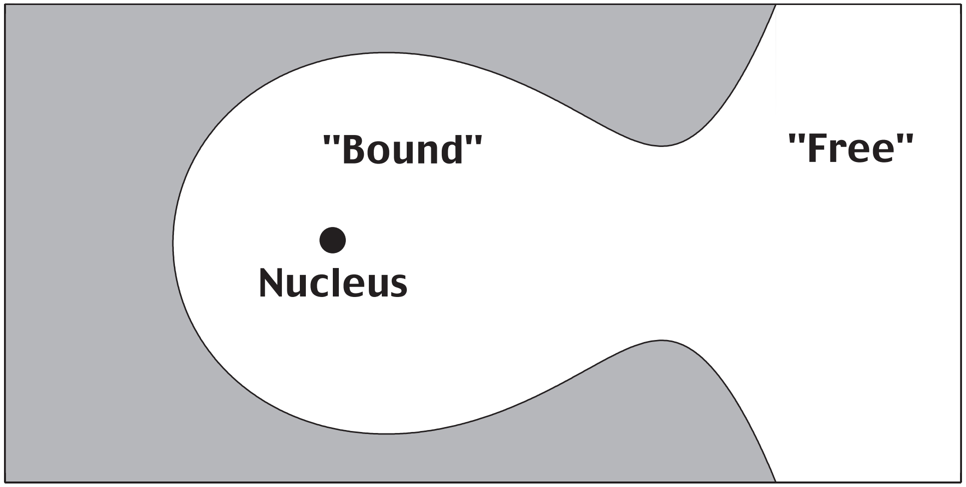


Partition the Phase Space

- ***Systems with potential barriers***
  - Electron near a nucleus



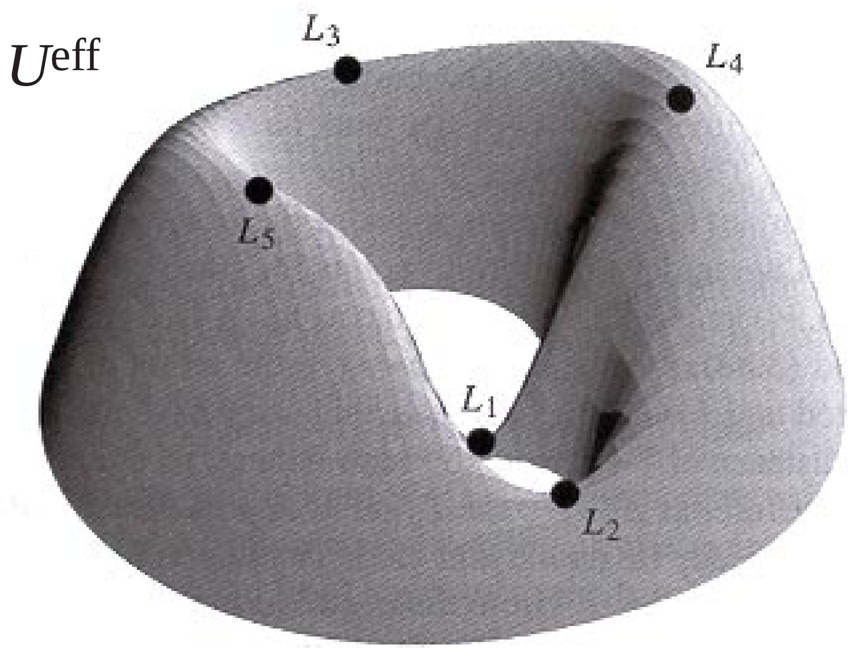
Potential



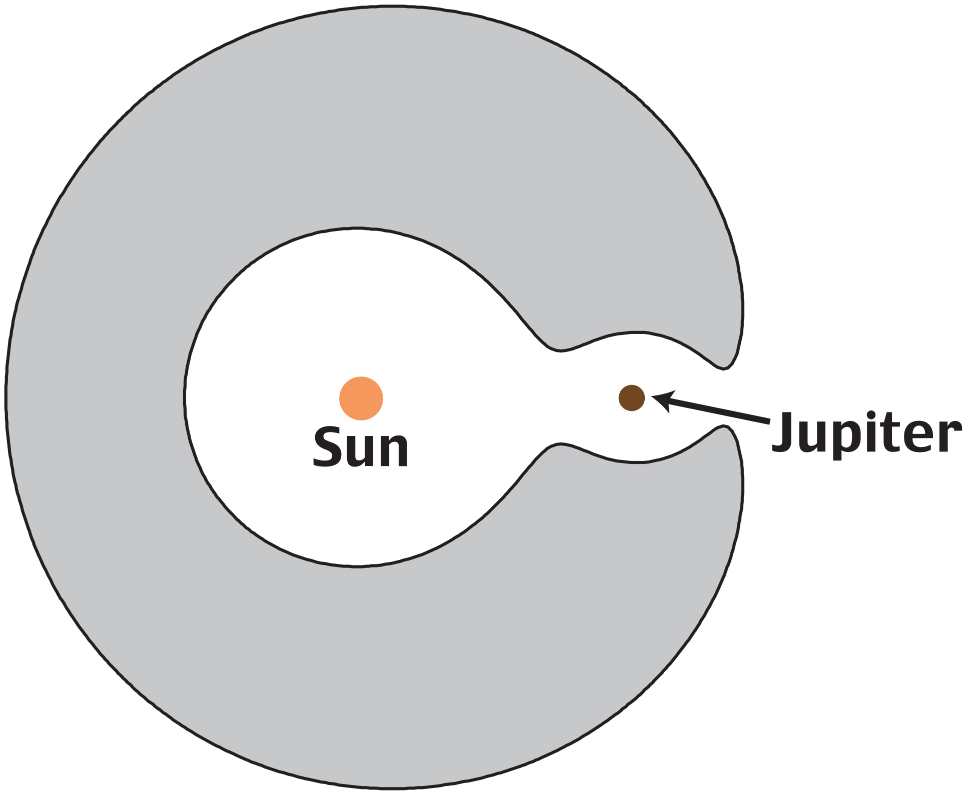
Configuration Space

Partition the Phase Space

- Comet near the Sun and Jupiter



Potential



Configuration Space

Partition the Phase Space

- ***Partition is specific to problem***
  - We desire a way of describing dynamical boundaries that represent the "frontier" between qualitatively different types of behavior
- ***Example: motion of comet***
  - motion around Sun
  - motion around Jupiter

Statement of Problem

- Suppose we study the motion on a manifold $\mathcal{M}$
- Suppose $\mathcal{M}$ is partitioned into disjoint regions

$$R_i, i = 1, \ldots, N_R,$$

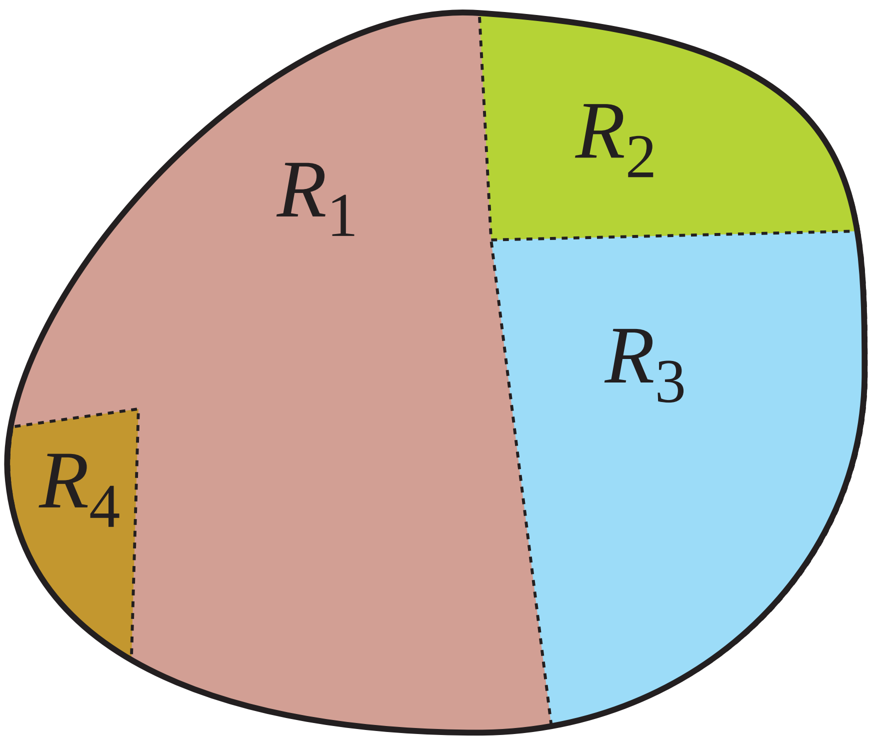
  such that

$$\mathcal{M} = \bigcup_{i=1}^{N_R} R_i.$$

- To keep track of the initial condition of a point, we say that *initially* (at $t = 0$) region R_i is uniformly covered with species S_i.
- Thus, species type of a point indicates the region in which it was located initially.

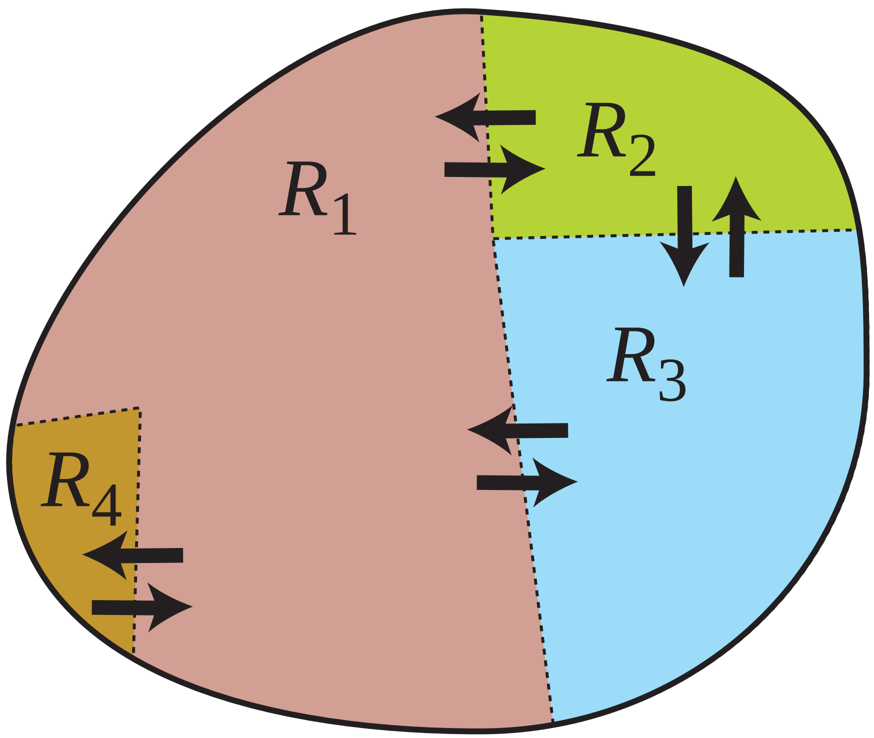
Statement of Problem

- Statement of the transport problem:
  Describe the distribution of species $S_i, i = 1, \ldots, N_R$, throughout the regions $R_j, j = 1, \ldots, N_R$, for any time $t > 0$.



Statement of Problem

- Some quantities we would like to compute are:
  - $T_{i,j}(t)$ = **the total amount of species S_i contained in region R_j at time t**
  - $F_{i,j}(t) = \frac{dT_{i,j}}{dt}(t)$ = **the flux of species S_i into region R_j at time t**



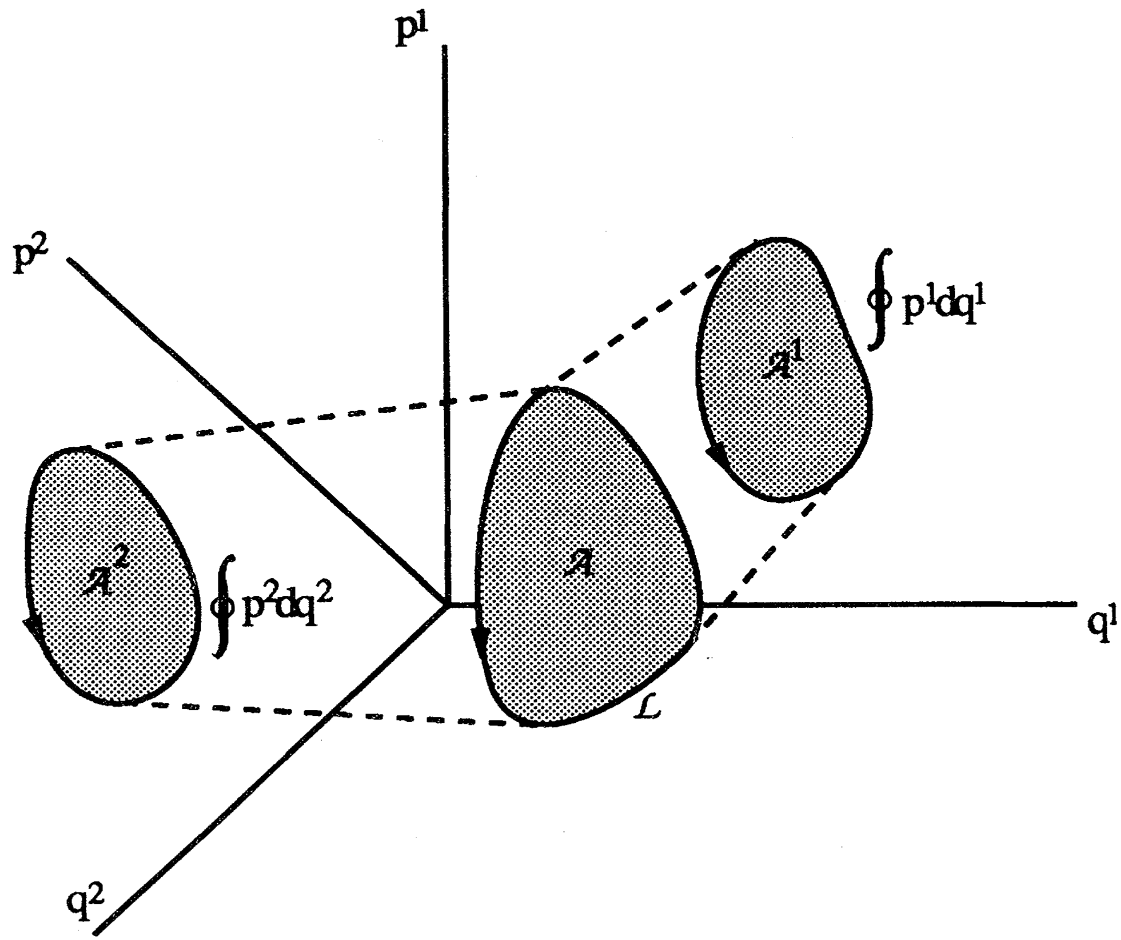
Hamiltonian Systems

- ***Time-independent Hamiltonian*** $H(q, p)$
  - N degrees of freedom
  - Motion constrained to a $(2N-1)$-dimensional energy surface $\mathcal{M}_E$ corresponding to a value $H(q,p) = E =$ constant
  - Symplectic area is conserved along the flow

$$\oint_{\mathcal{L}} p \cdot dq = \int_{\mathcal{A}} dp \wedge dq = \text{constant}$$

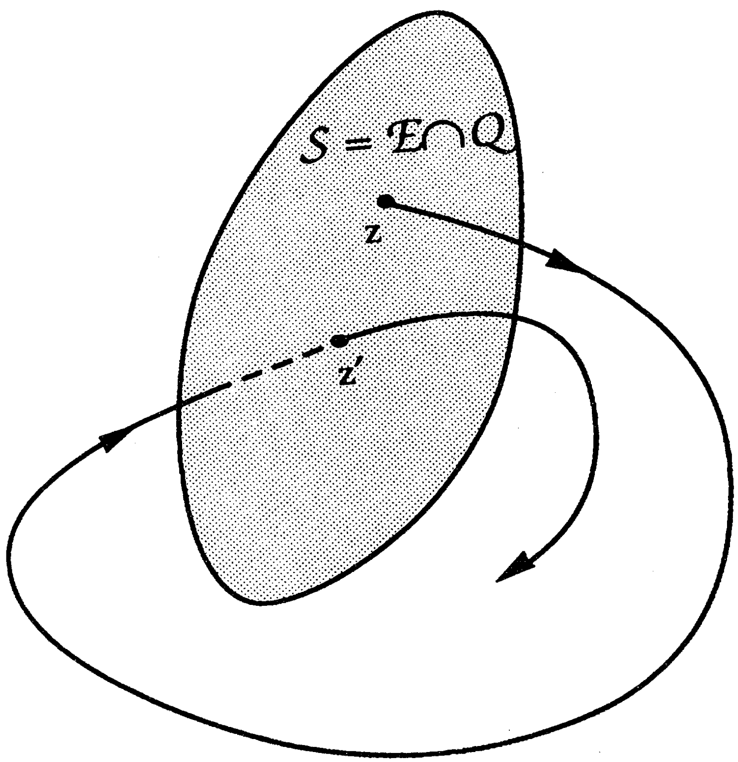
Symplectic Area Conserved

$$\sum_{i=1}^{N} \sigma_i \int_{\mathcal{A}^i} dp_i dq^i = \text{constant on an energy surface}$$



Poincaré Section

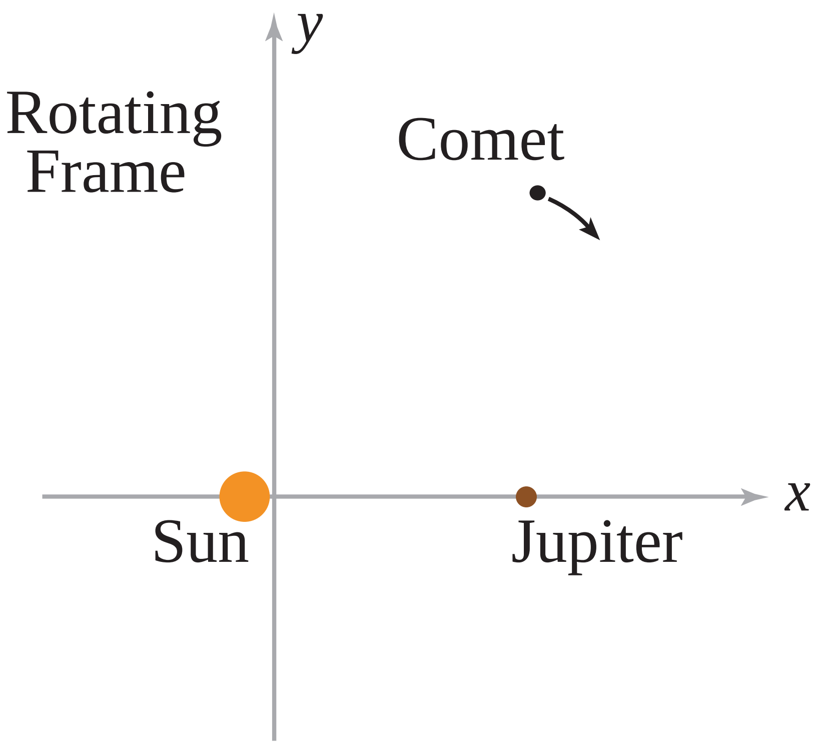
- Suppose there is another $(2N-1)$-dimensional surface $\mathcal{Q}$ that is transverse (i.e., nowhere parallel) to the flow in some local region.
- The Poincaré section $\mathcal{S}$ is the $(2N-2)$-dimensional intersection of $\mathcal{M}_E$ with $\mathcal{Q}$.



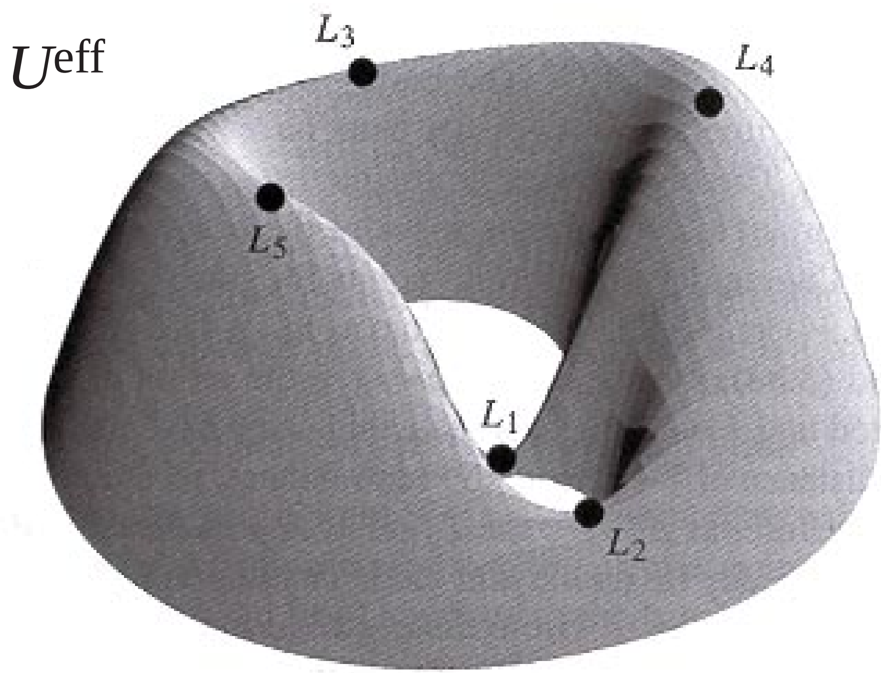
Example for $N = 2$

- ***Circular restricted 3-body prob. (2D)***

$$H = \frac{1}{2}((p_x + y)^2 + (p_y - x)^2) + U^{\text{eff}}(x, y)$$



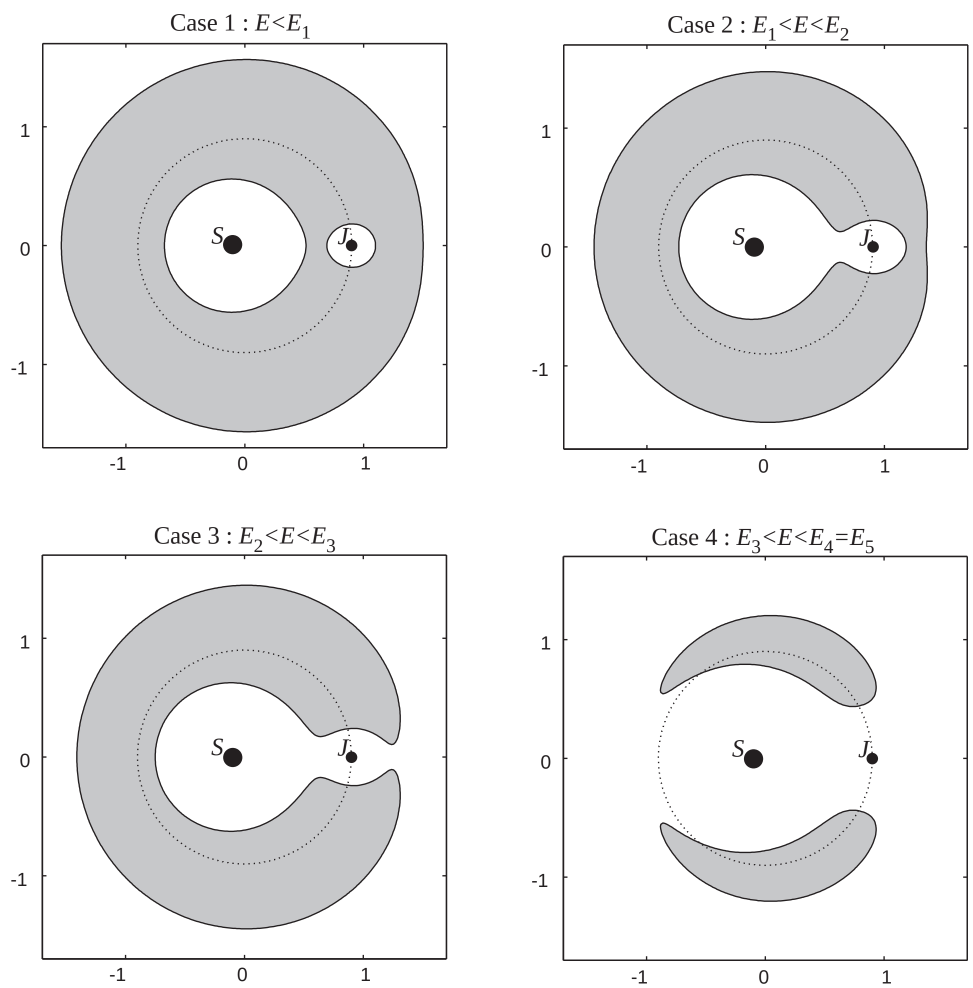
Position Space



Effective Potential

3-Body Problem (2D)

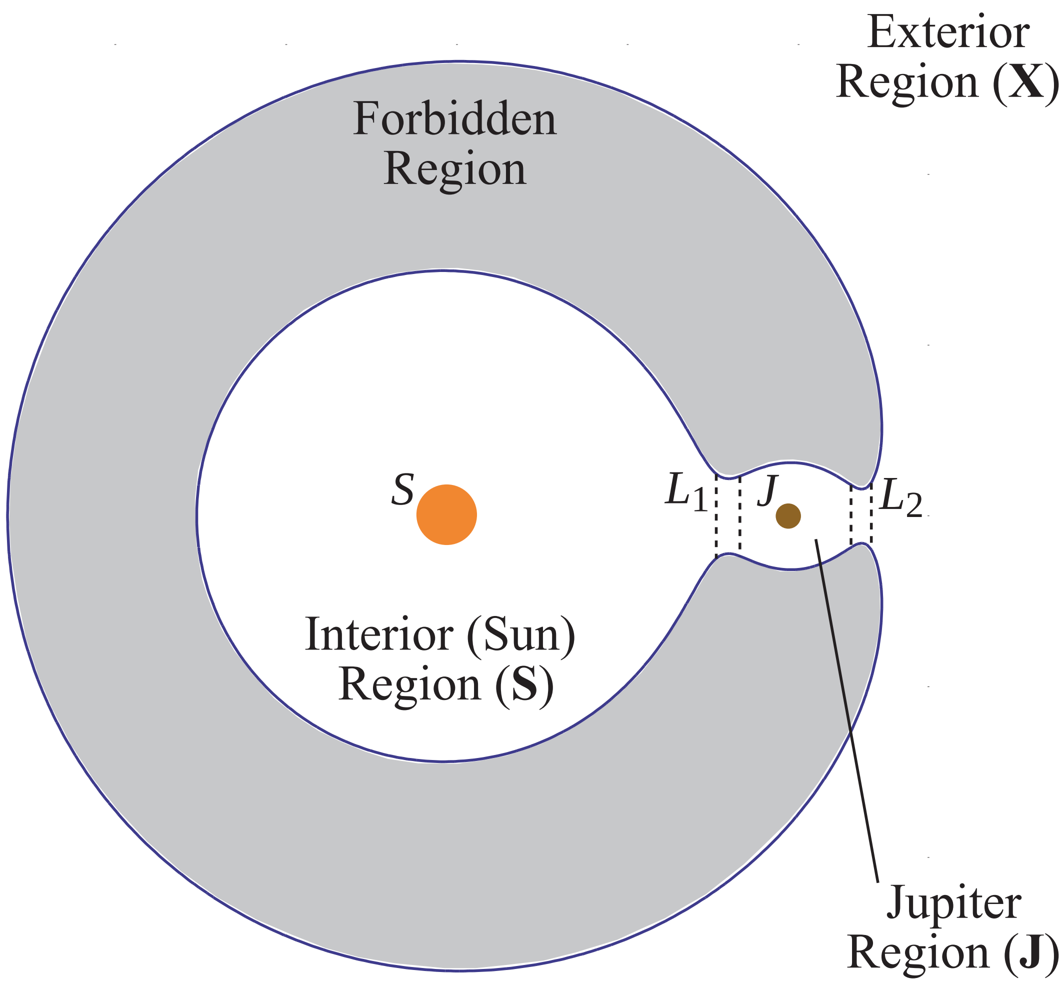
- ***Look at fixed energy***



Position Space Projections

3-Body Problem (2D)

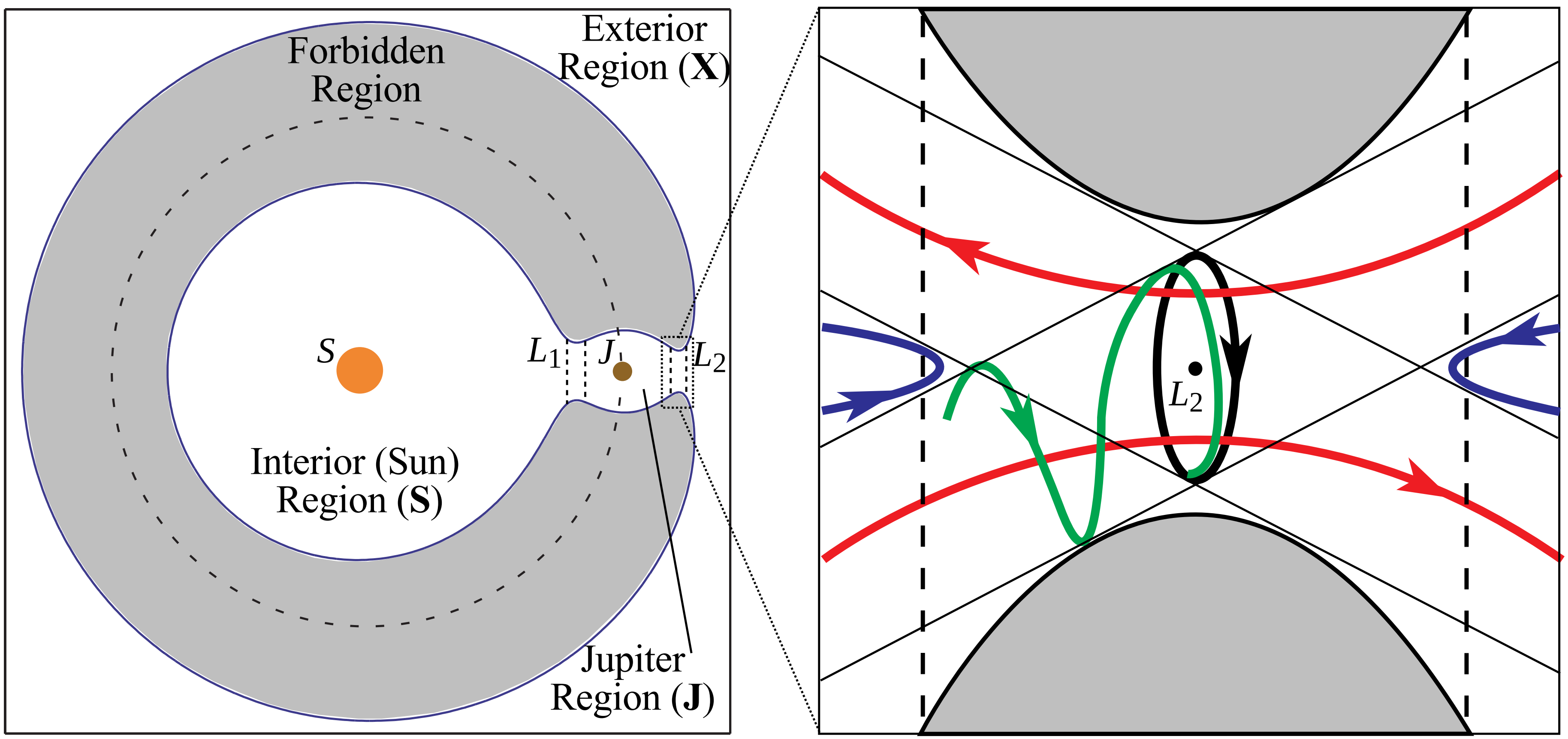
- ***Partition the energy surface***



Position Space Projection

3-Body Problem (2D)

- ***Look at motion near "saddle points"***



Position Space Projection

Potential Barriers

- Hamiltonian systems with potential barriers give rise to "saddle points" whose local form is given by

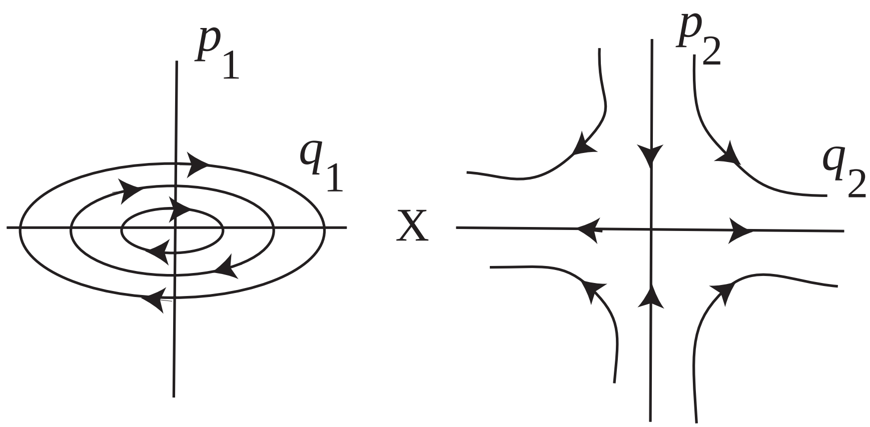
$$H(q,p) = \frac{\omega}{2}(q_1^2 + p_1^2) + \lambda q_2 p_2, \qquad (1)$$

i.e., linearized vector field has eigenvalues $\pm i\omega$, $\pm\lambda$.

- Moser [1958] showed that the qualitative behavior of (1) carries over to the full nonlinear equations.
- In particular, the flow of (1) has form center $\times$ saddle.

Local Dynamics

- For fixed energy $H = h$, energy surface $\simeq S^2 \times \mathbb{R}$.
- Other constants of motion: $I_1 = q_1^2 + p_1^2$ and $I_2 = q_2 p_2$.



- Normally hyperbolic invariant manifold at $q_2 = p_2 = 0$, i.e.,

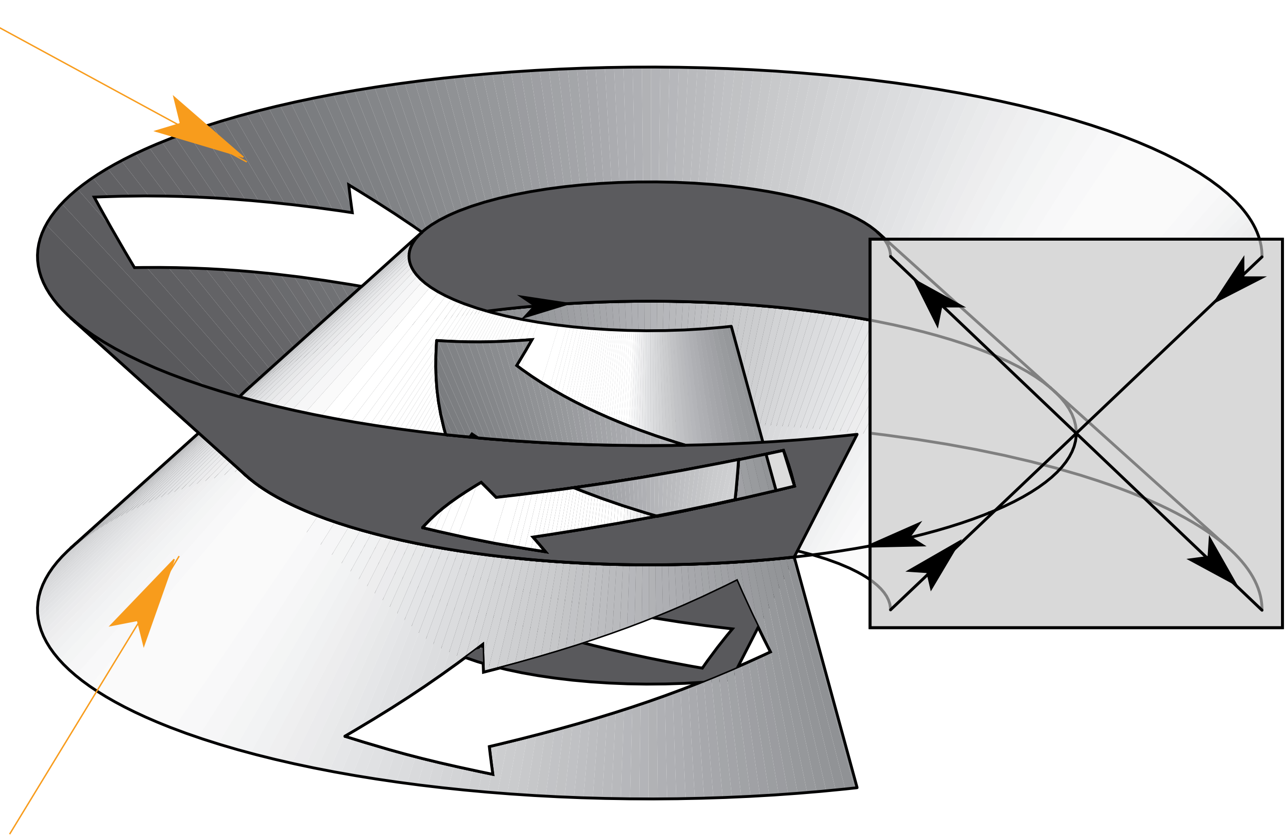
$$\mathcal{M}_h = \frac{\omega}{2}(q_1^2 + p_1^2) = h > 0.$$

Note that $\mathcal{M}_h \simeq S^1$, a periodic orbit.

Local Dynamics

- Four cylinders of asymptotic orbits: the stable and unstable manifolds $W^s_\pm(\mathcal{M}_h), W^u_\pm(\mathcal{M}_h)$.

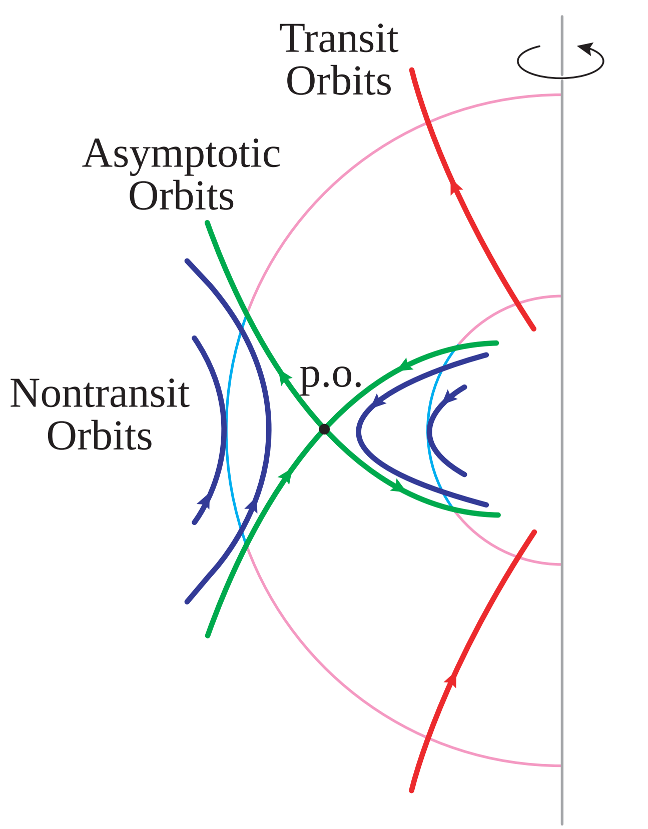
Stable Manifold (orbits move toward the periodic orbit)



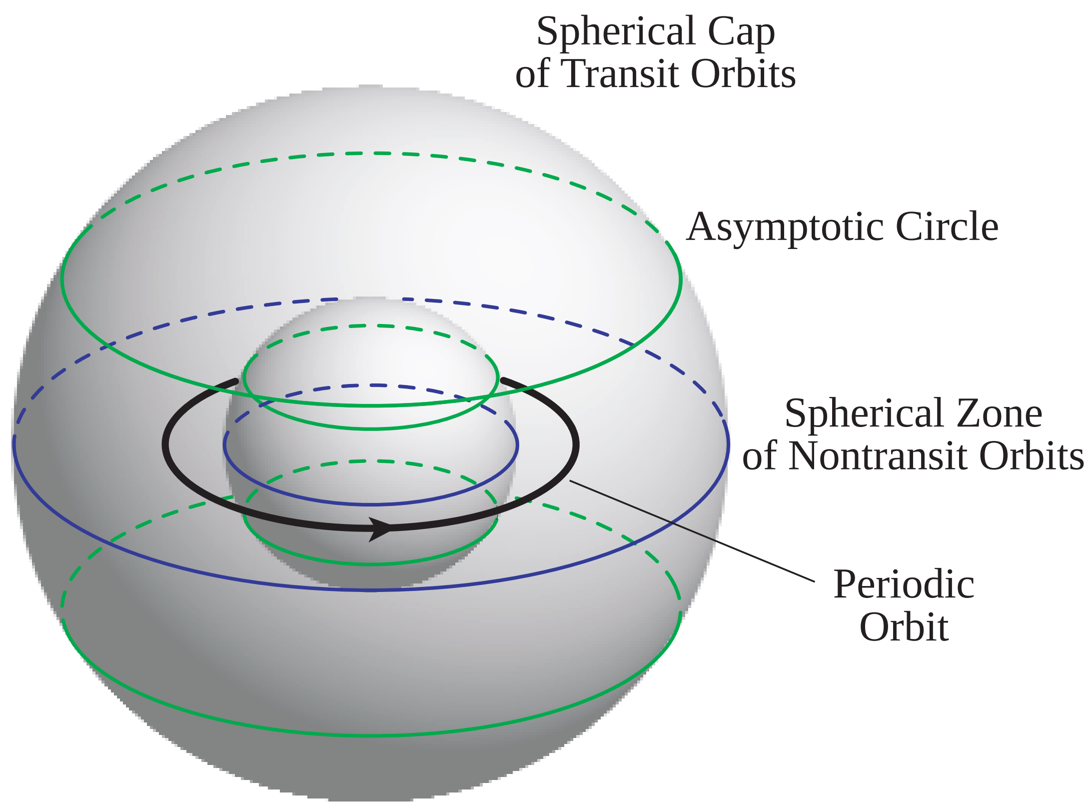
Unstable Manifold (orbits move away from the periodic orbit)

Transit and Nontransit Orbits

- Cylinders separate transit from nontransit orbits.
- Define mappings between “bounding spheres” on either side of the potential barrier.



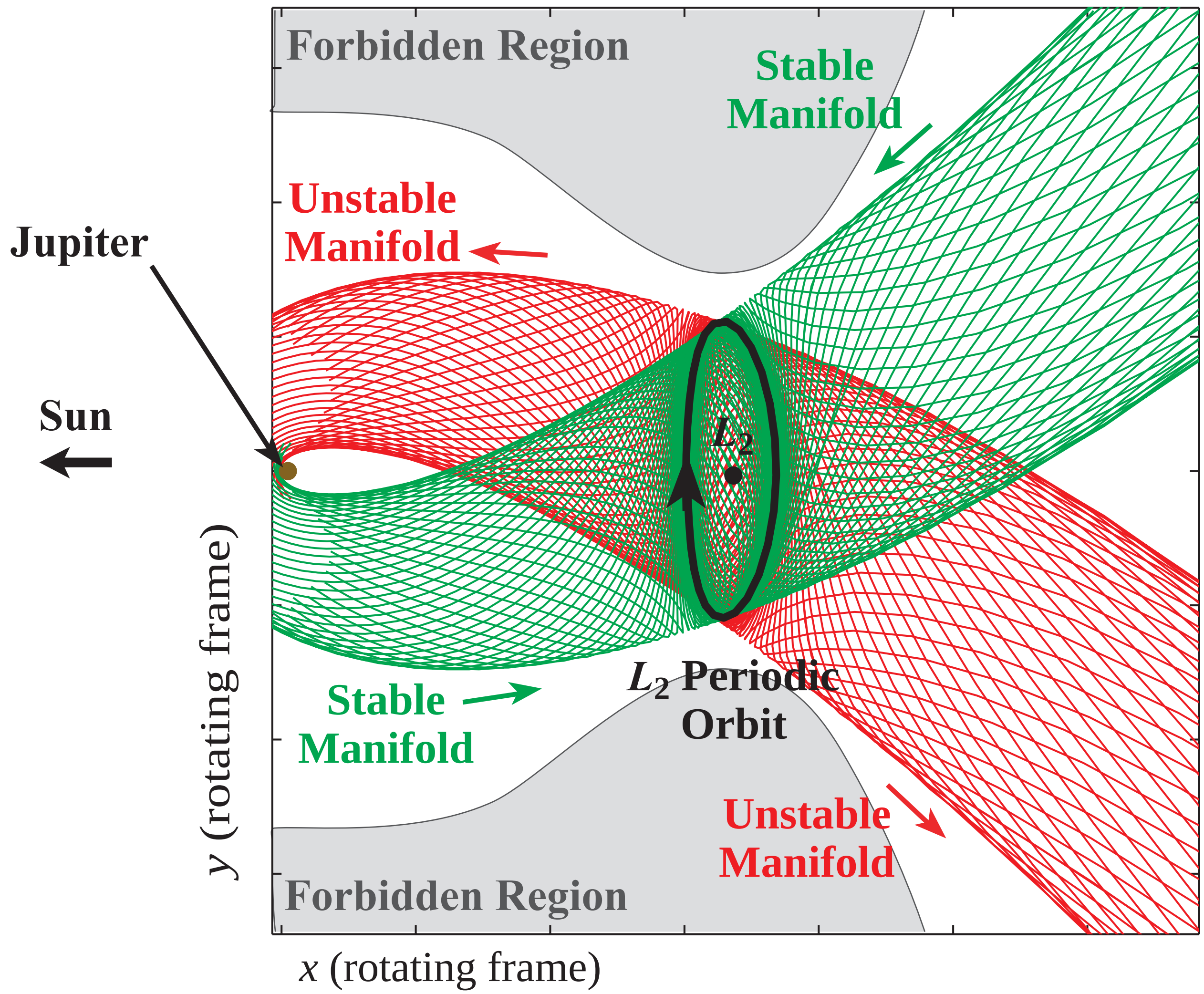
Cross-section of Equilibrium Region



Equilibrium Region

Tubes in the 3-Body Problem

- **Stable** and **unstable** manifold tubes
  - Control transport through the potential barrier.

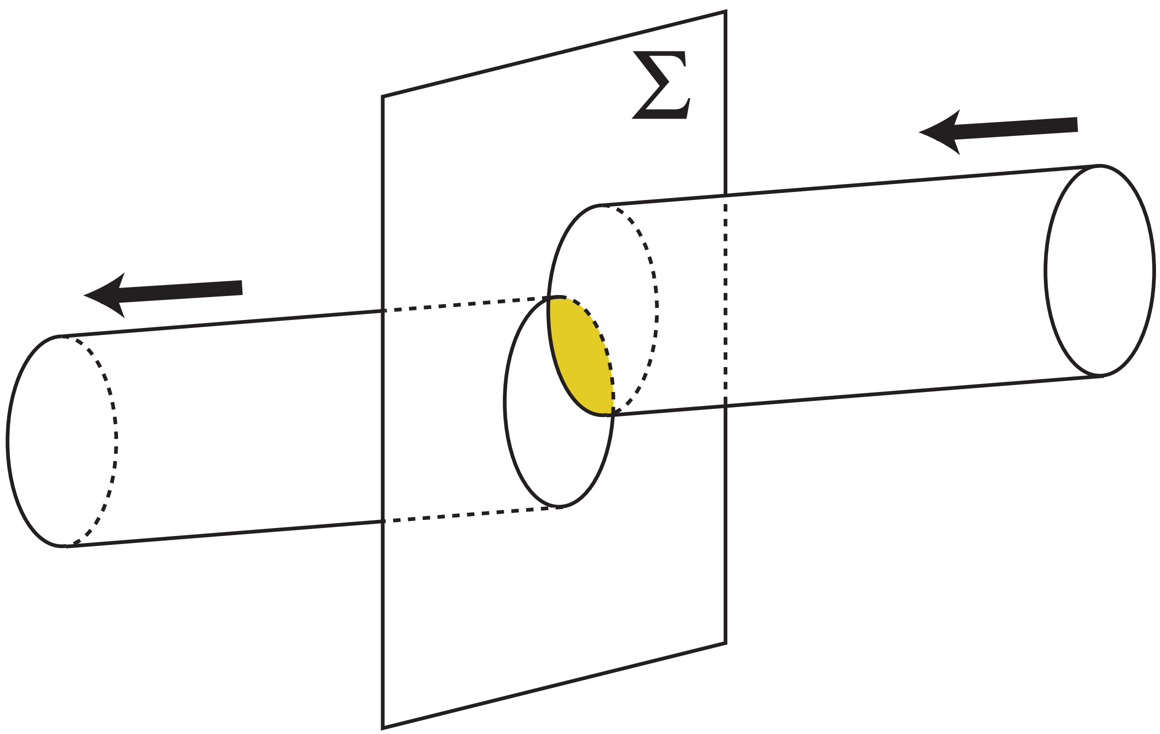


Flux

- ***Tubes of transit orbits are the relevant objects to study***
  - Tubes determine the flux between regions $F_{i,j}(t)$.
  - Note, net flux is zero for volume-preserving motion, so we consider the one-way flux.
    - **Example: $F_{J,S}(t)$ = volume of trajectories that escape from the Jupiter region into the Sun region per unit time.**

Transition Probablities

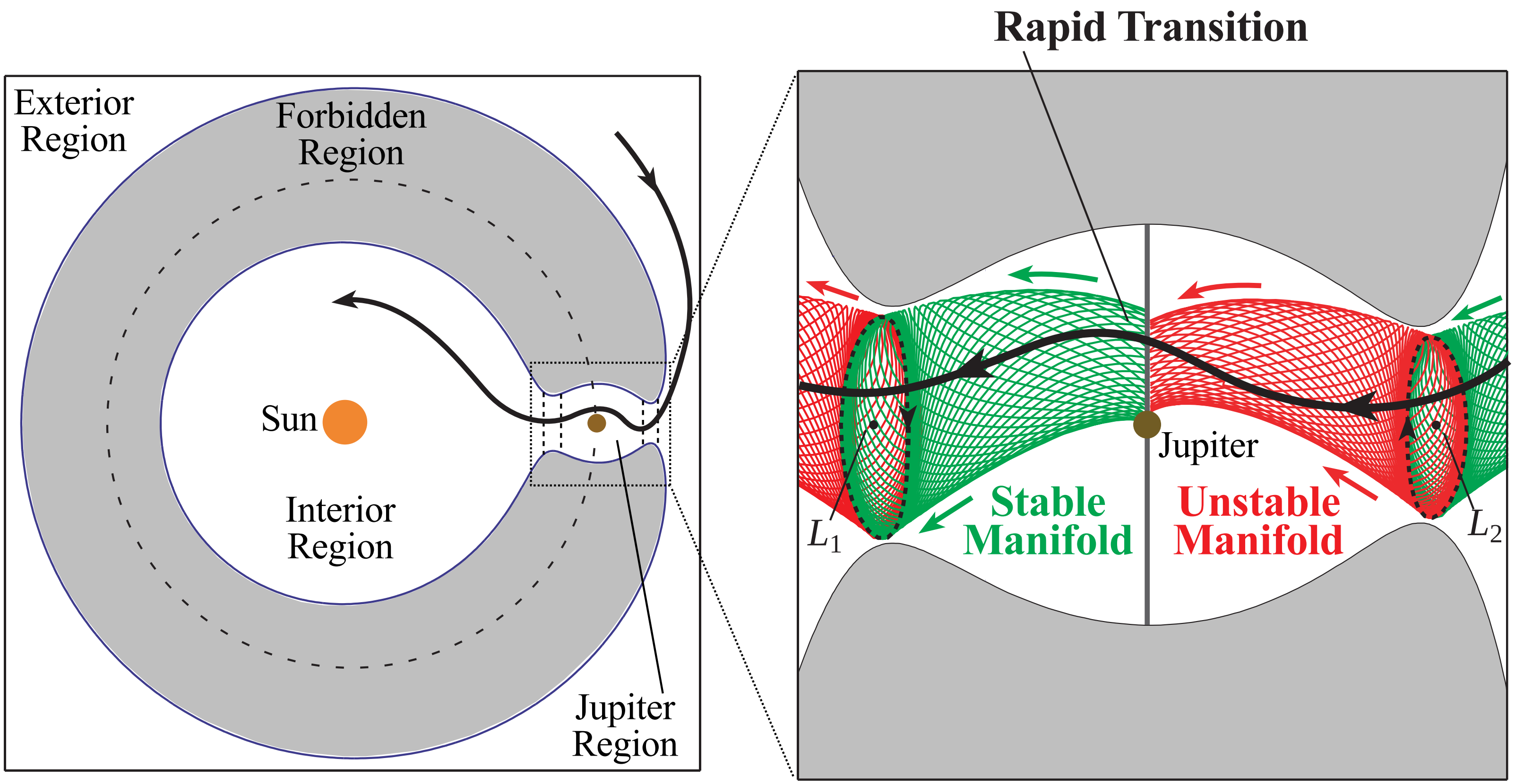
- ***More exotic transport between regions***
  - Look at the intersections between the interior of stable and unstable tubes on the same energy surface.
  - Could be from different potential barrier saddles.



Poincaré Section

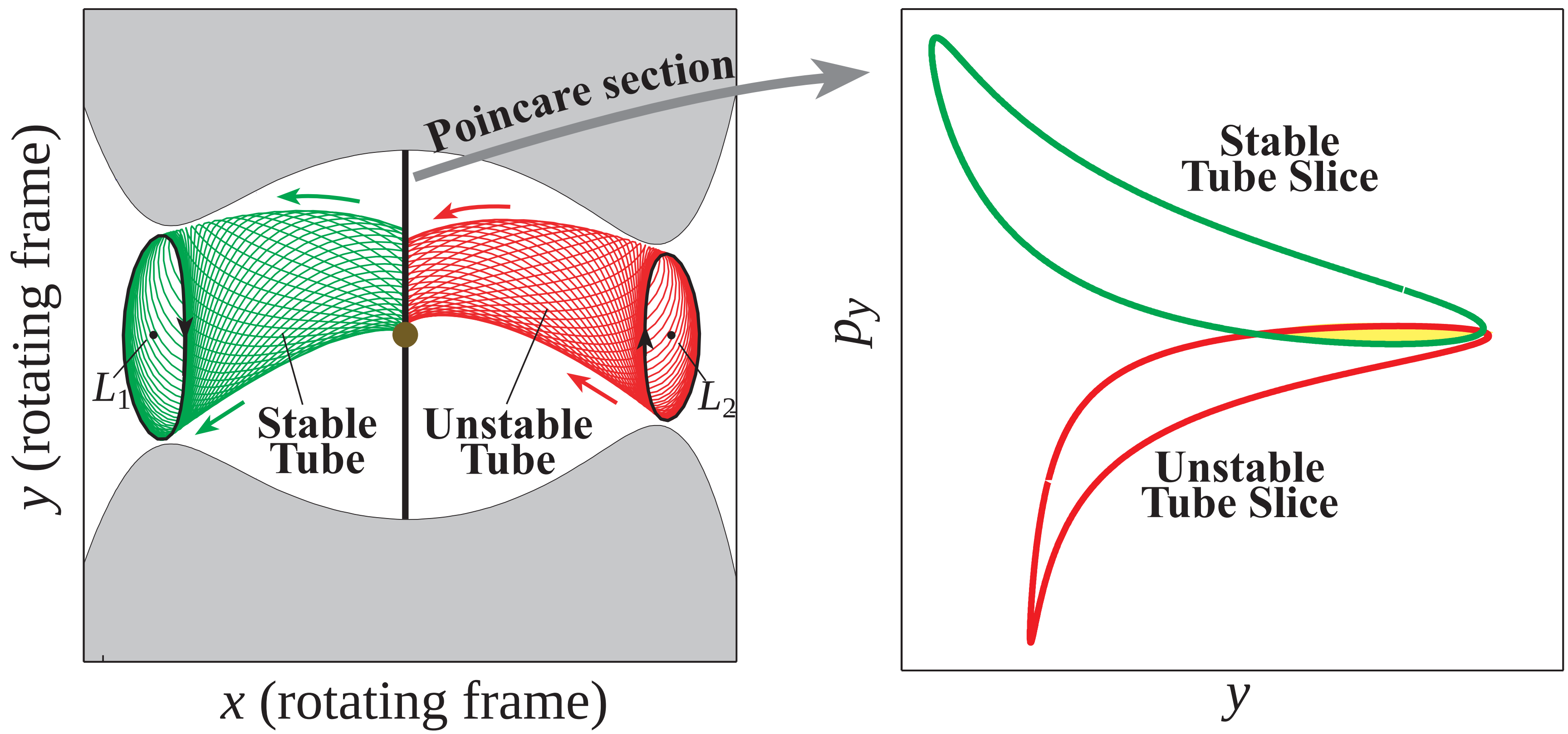
Transition Probablities

- Example: Comet transport between outside and inside of Jupiter



Transition Probablities

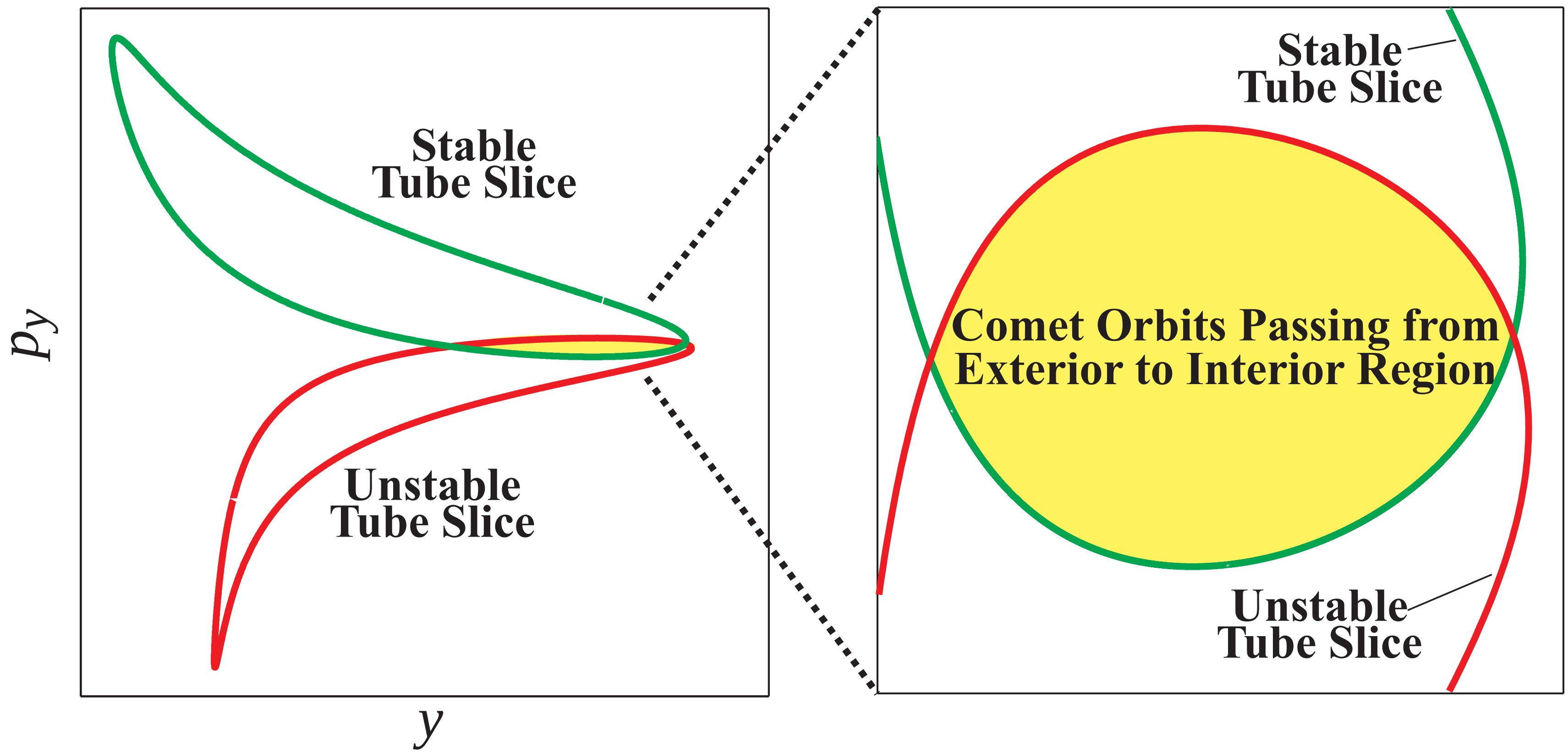
- Look at Poincaré section intersected by both tubes.
- Choosing surface $\{x = \text{constant}; p_x < 0\}$, we look at the canonical plane (y, p_y).



Position Space **Canonical Plane (y, p_y)**

Transition Probablities

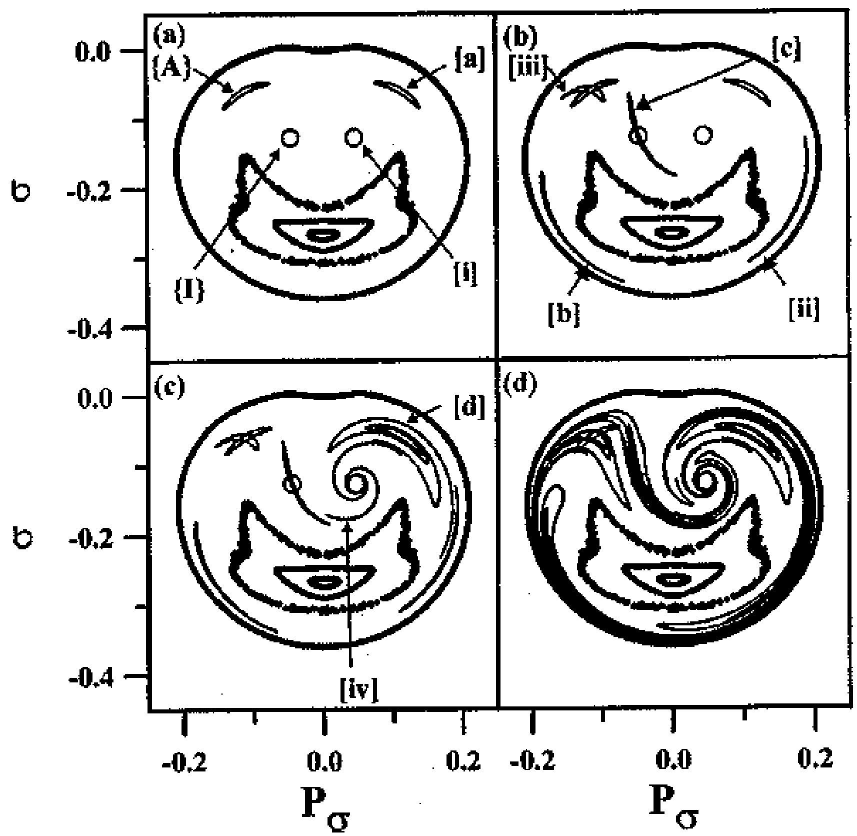
- Relative canonical area gives relative volume of orbits.
- Under certain ergodic assumptions, the relative volume can be interpreted as the probability of transition.



Canonical Plane (y, p_y)

Mixing

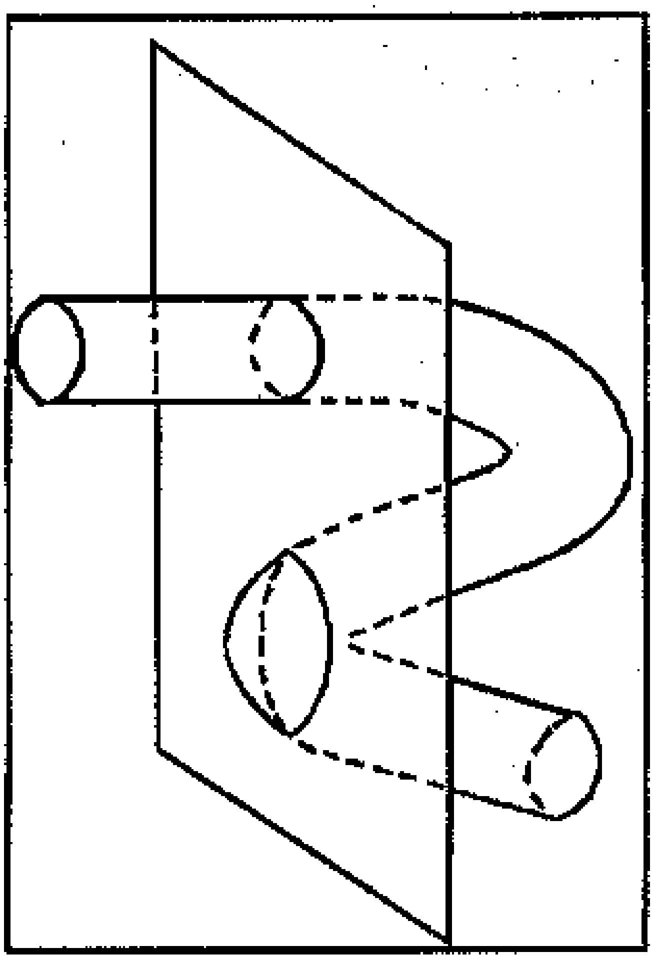
- By keeping track of the intersections of the tubes, one can describe the mixing of different regions ($T_{i,j}(t)$).
  - **It can get messy fast!**



(from Jaffé, Farrelly and Uzer [1999])

Some Challenges

- Computationally very challenging
- How to handle non-transversal intersections



$N = 3$ or More

- ***Extend to $N \geq 3$ degrees of freedom***
  - Near equilibrium point, suppose linearized Hamiltonian vector field has eigenvalues $\pm i\omega_j$, $j = 1, \ldots, N-1$, and $\pm\lambda$.
  - Assume the complexification is diagonalizable.
  - Hamiltonian normal form theory tranforms Hamiltonian into a lowest order form:

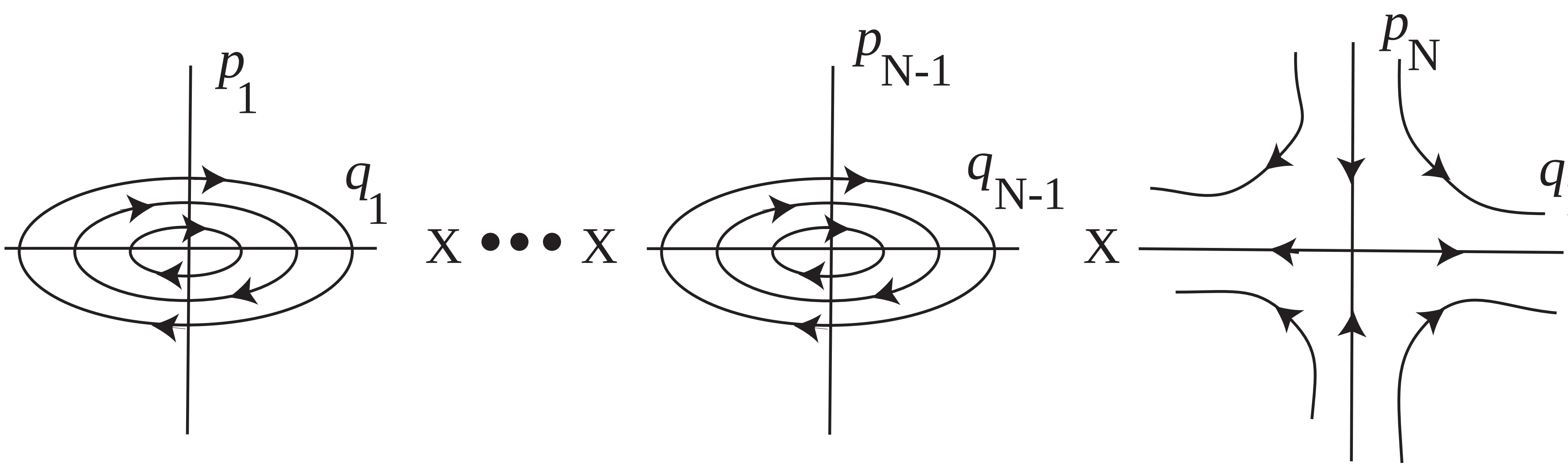
$$H(q,p) = \sum_{i=1}^{N-1} \frac{\omega_i}{2}\left(p_i^2 + q_i^2\right) + \lambda q_N p_N.$$

  - Equilibrium point is of type center $\times \cdots \times$ center $\times$ saddle ($N-1$ centers).

$N = 3$ or More

Multidimensional "saddle point"

- For fixed energy $H = h$, energy surface $\simeq S^{2N-2} \times \mathbb{R}$.
- Constants of motion:
  $I_j = q_j^2 + p_j^2, j = 1, \ldots, N-1$, and $I_N = q_N p_N$.



The N Canonical Planes

$N = 3$ or More

- Normally hyperbolic invariant manifold at $q_N = p_N = 0$,

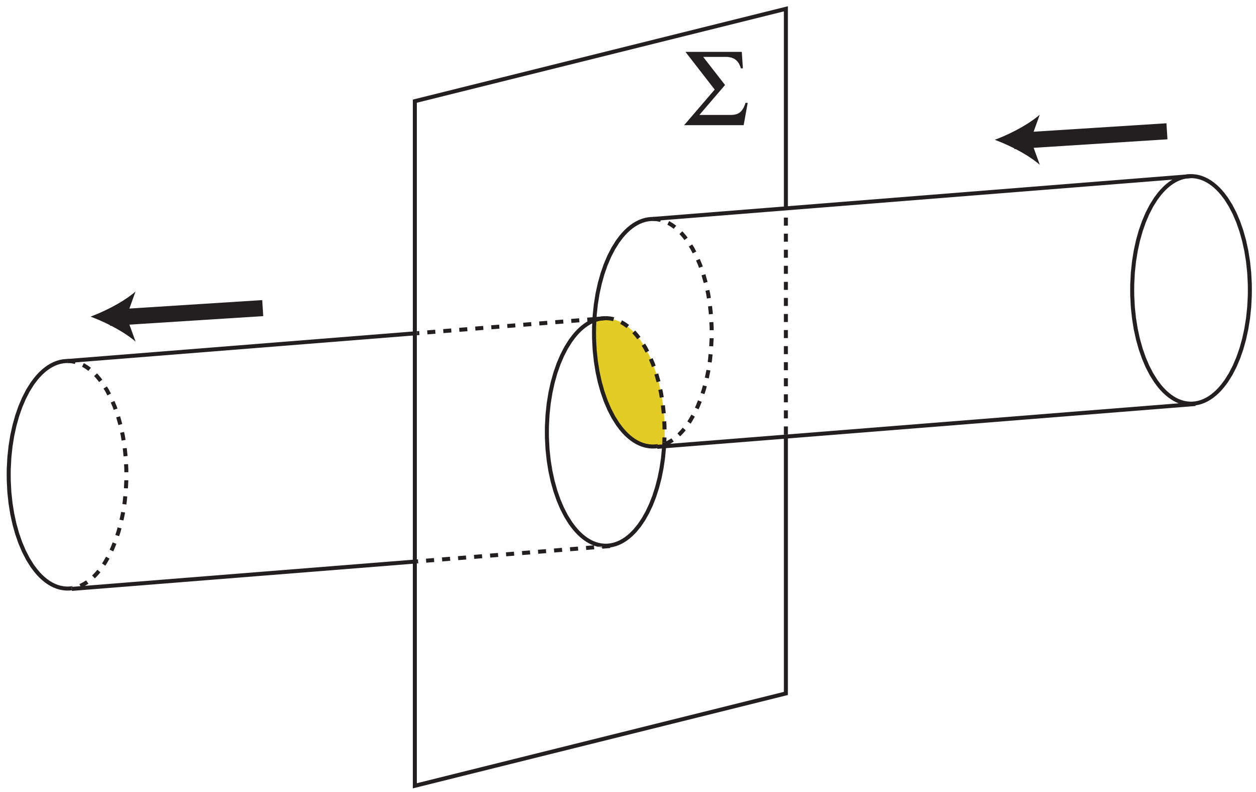
$$\mathcal{M}_h = \sum_{i=1}^{n-1} \frac{\omega_i}{2} \left(p_i^2 + q_i^2\right) = h > 0.$$

Note that $\mathcal{M}_h \simeq S^{2N-3}$, not a single trajectory.

- Four "cylinders" of asymptotic orbits: the stable and unstable manifolds $W^s_{\pm}(\mathcal{M}_h), W^u_{\pm}(\mathcal{M}_h)$, which have the structure $S^{2N-3} \times \mathbb{R}$.

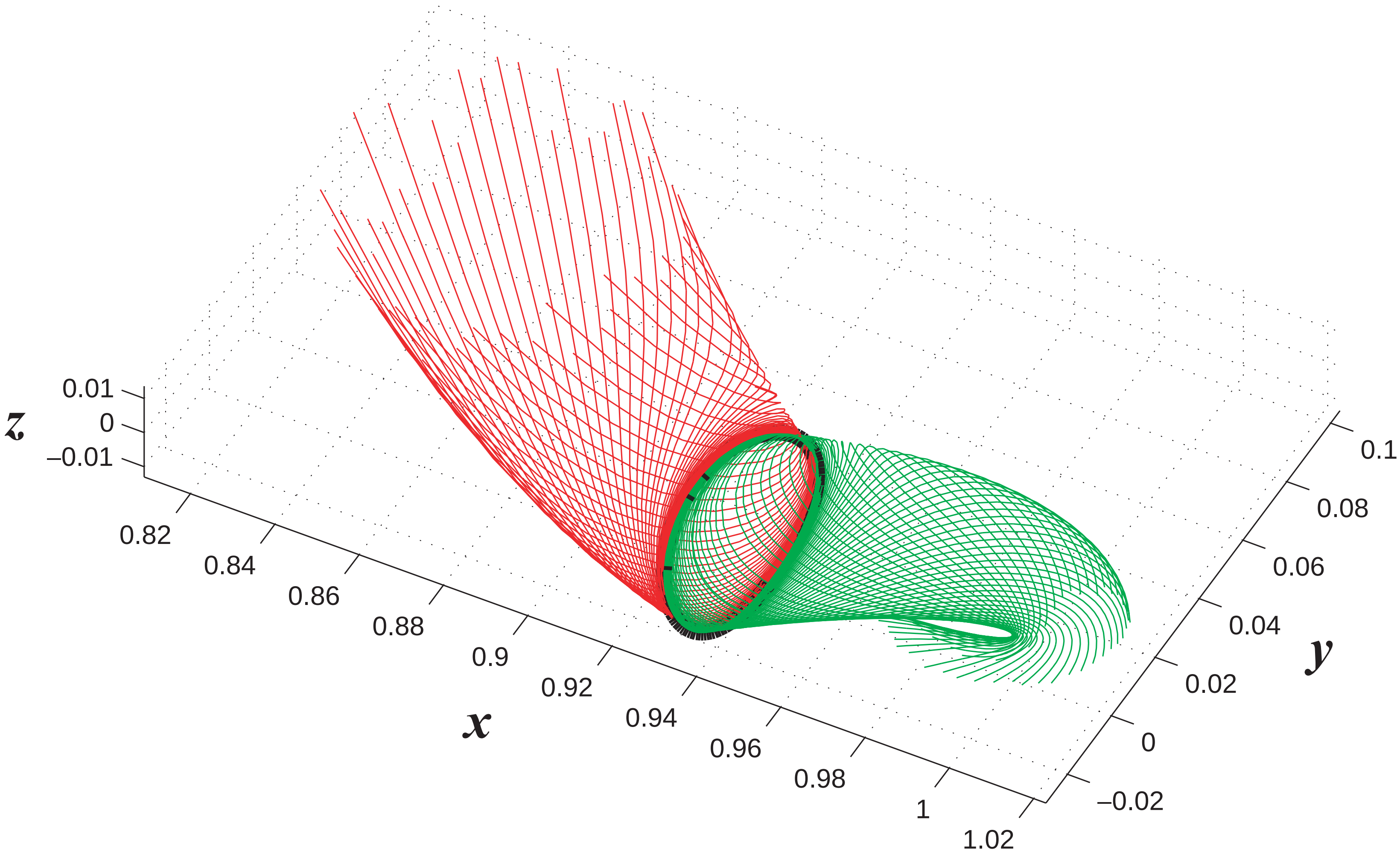
$N = 3$ or More

- Transport between regions is mediated by the "higher dimensional tubes"
- Compute fluxes, transition probabilities, etc.



$N = 3$ or More

- Example: restricted three-body problem (3D)



3D Position Space

Future Directions

- Future Directions
  - **Compute fluxes, transition probabilities in 2 and 3 degree of freedom systems**
  - **Determine statistical laws**
    - For one energy
    - Over a range of energies
    - Is ergodic assumption valid?
    - Equilibrium distribution?
    - Relaxation time to equilibrium?
  - **Apply to astronomical and chemical systems**
    - Astronomy: Compute asteroid collision probabilities, "equilibrium" distribution of asteroids and comets
    - Chemistry: Compute reaction rates
  - **Combine with control**

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