

Transport in Hamiltonian Systems With Two or More Degrees of Freedom

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CDS

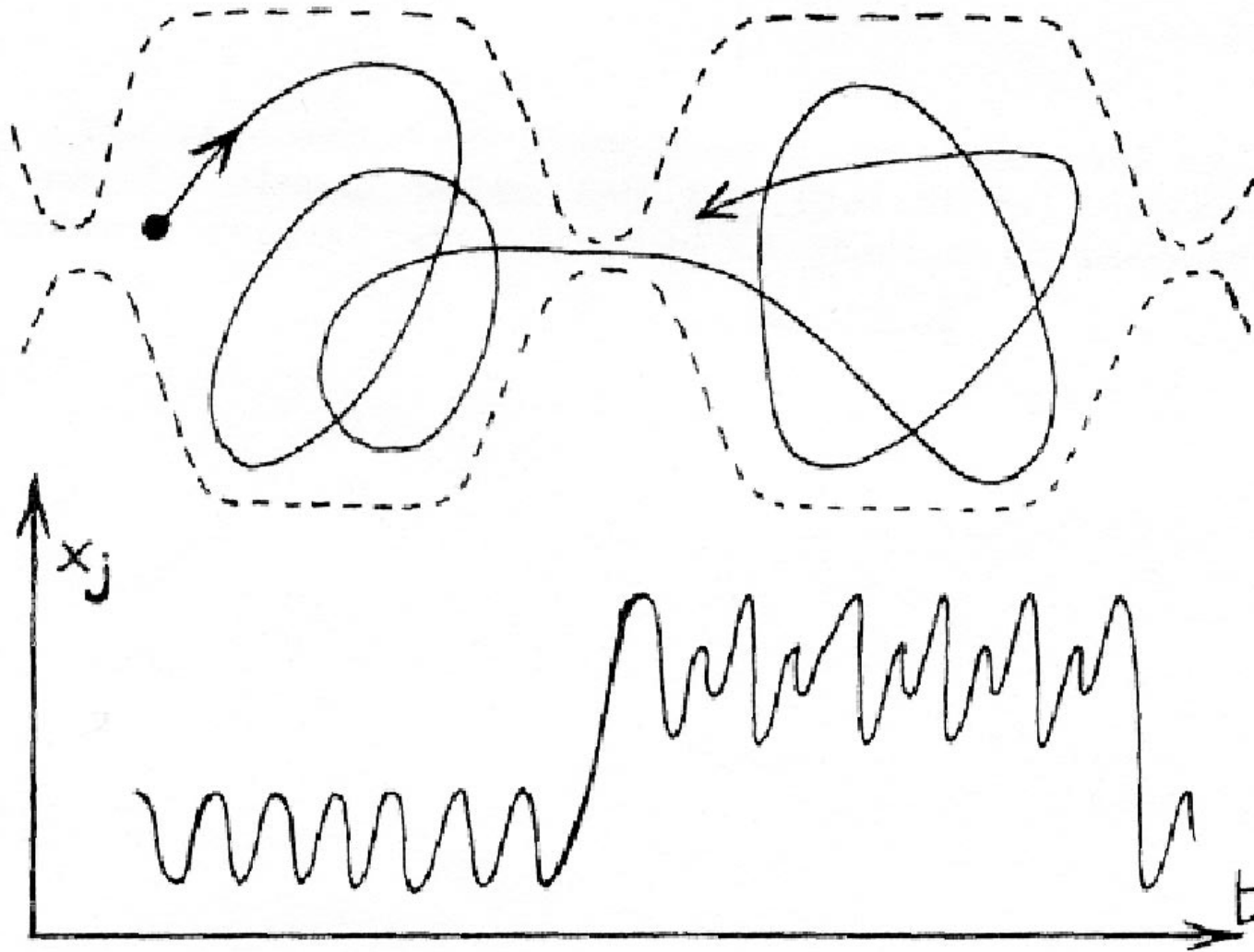
Control and Dynamical Systems

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*

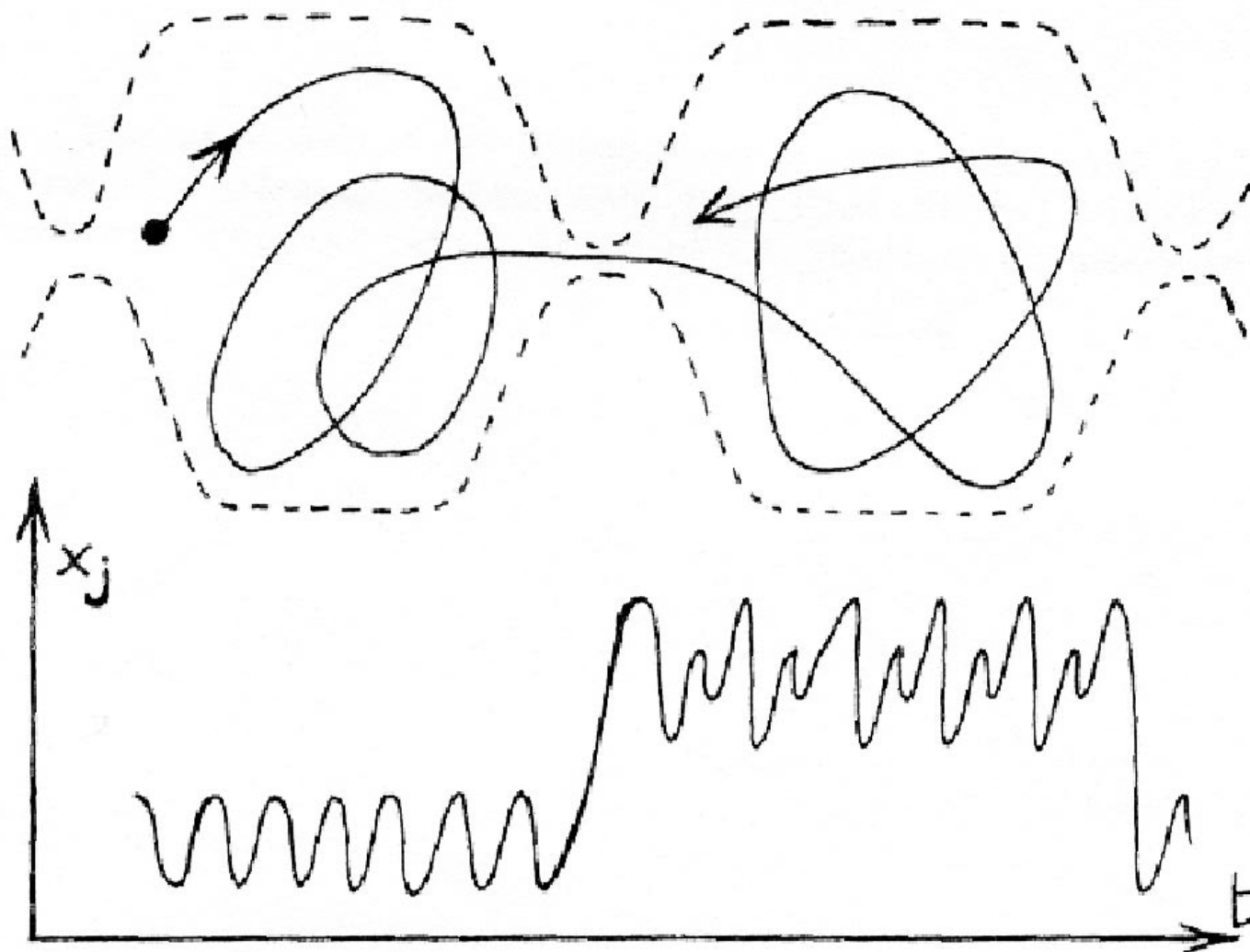
■ *Transport theory*

- 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

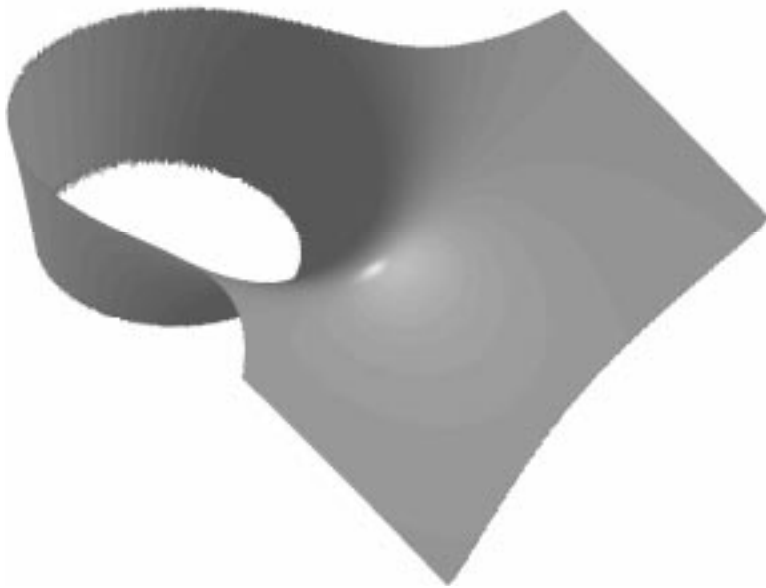
“Reactants”

“Products”

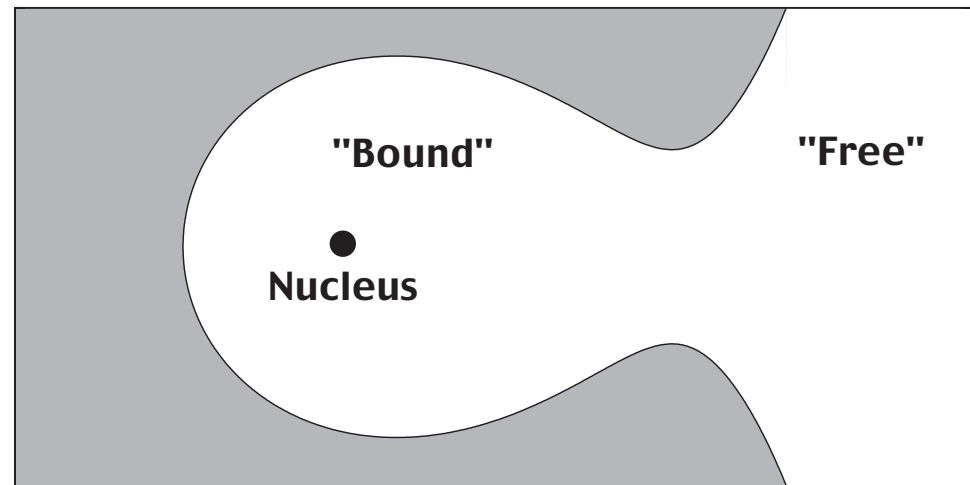


Partition the Phase Space

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



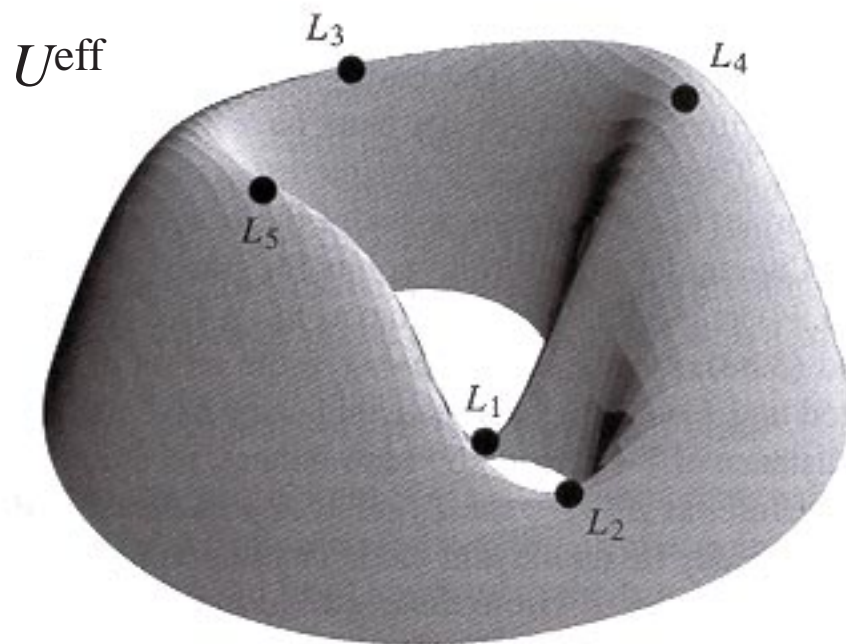
Potential



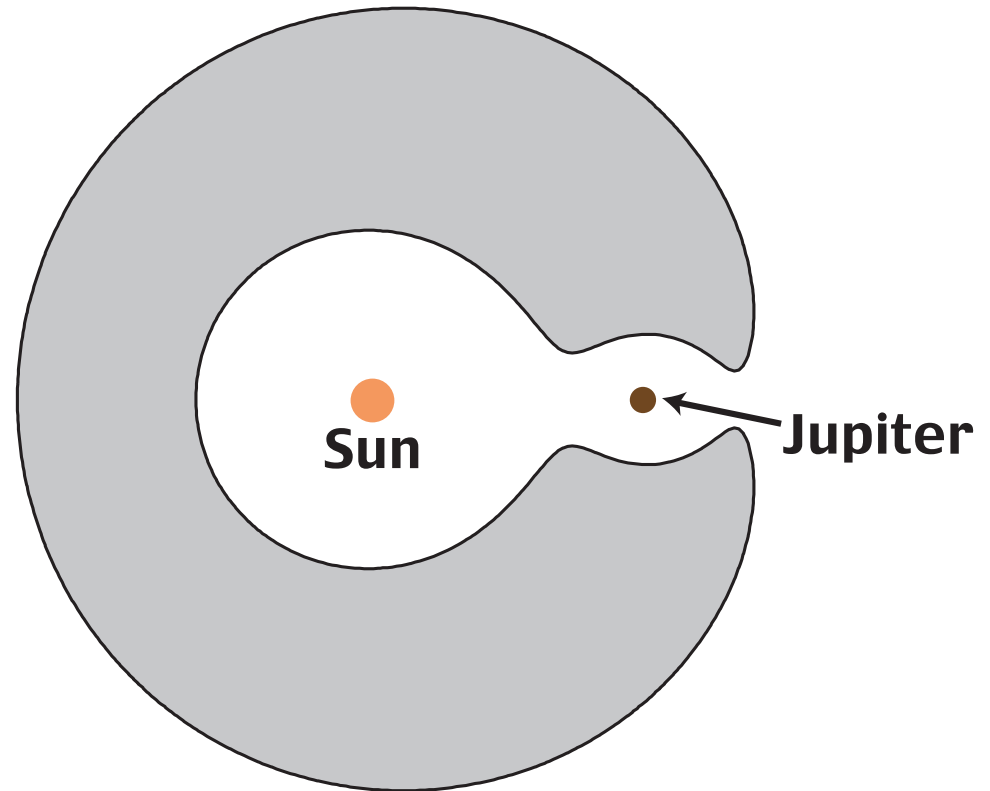
Configuration Space

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

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

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.

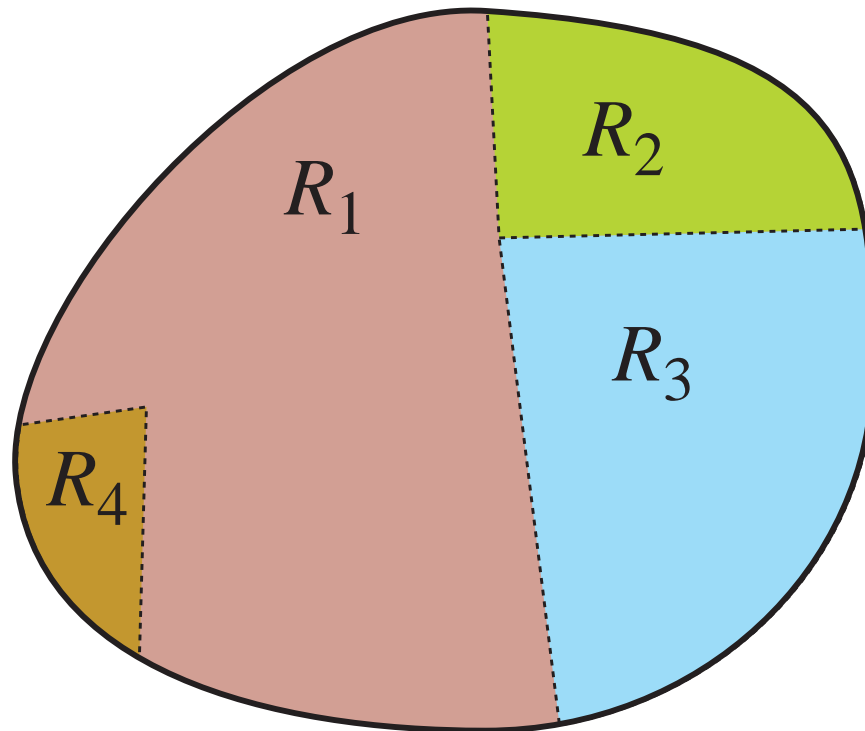
Statement of Problem

- Statement of the transport problem:

Describe the distribution of species

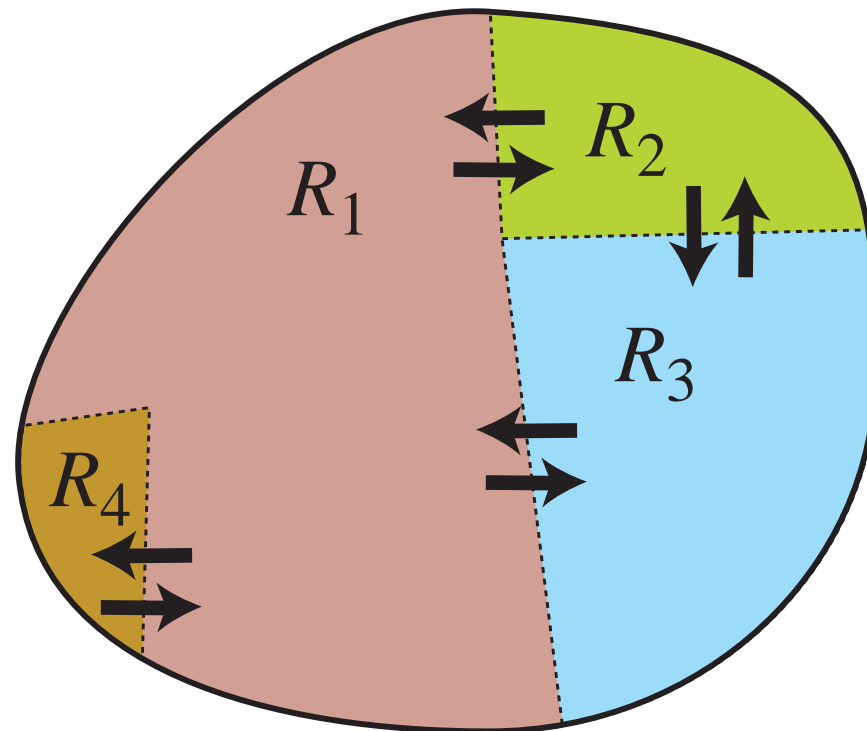
$S_i, i = 1, \dots, N_R$, **throughout the regions**

$R_j, j = 1, \dots, N_R$, **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

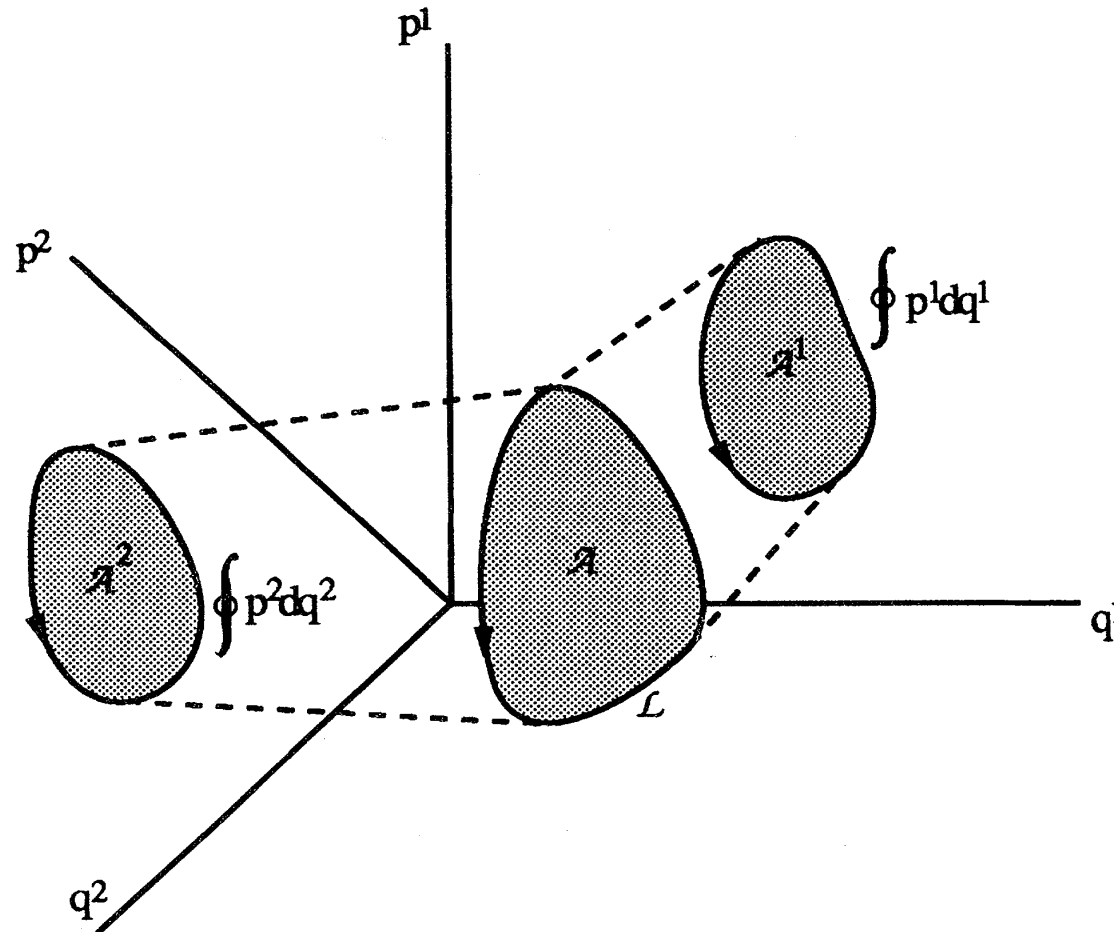
■ *Time-independent Hamiltonian* $H(q, p)$

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

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

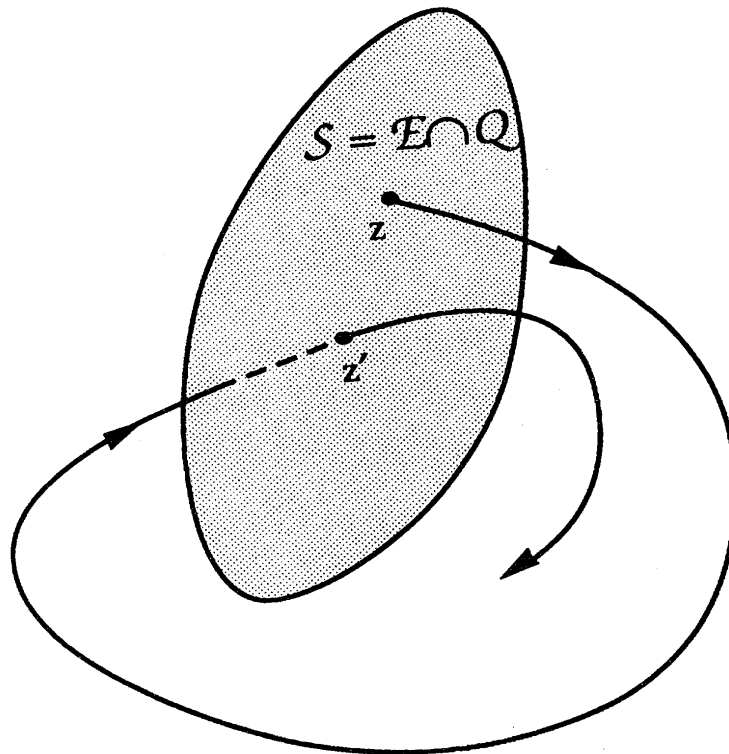
Symplectic Area Conserved

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



Poincaré Section

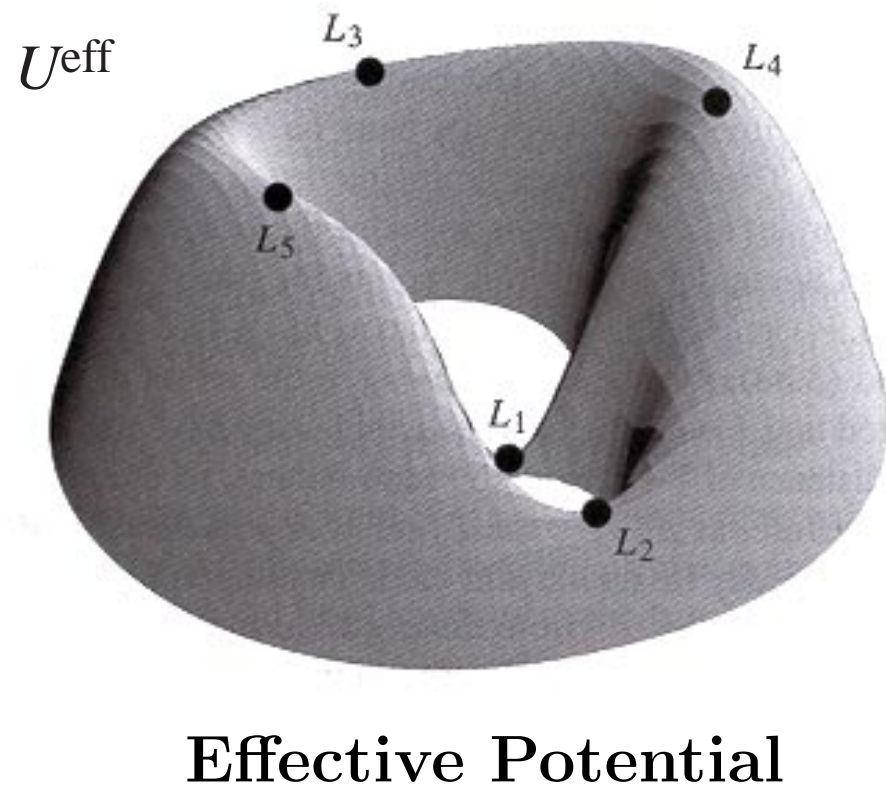
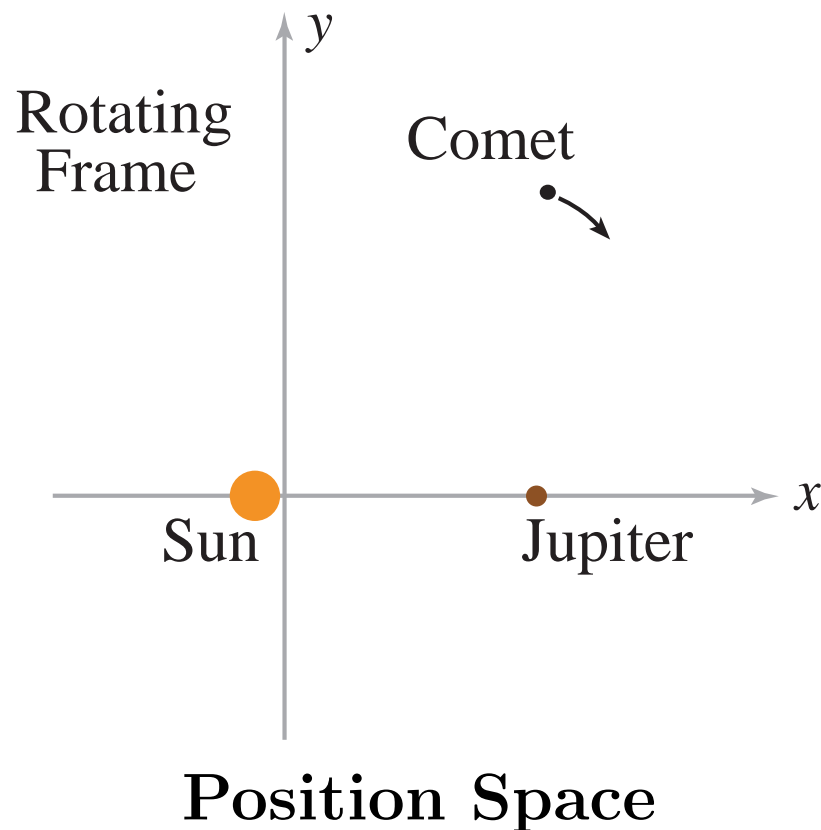
- Suppose there is another $(2N - 1)$ -dimensional surface \mathcal{Q} that is transverse (i.e., nowhere parallel) to the flow in some local region.
- The Poincaré section \mathcal{S} is the $(2N - 2)$ -dimensional intersection of \mathcal{M}_E with \mathcal{Q} .



Example for $N = 2$

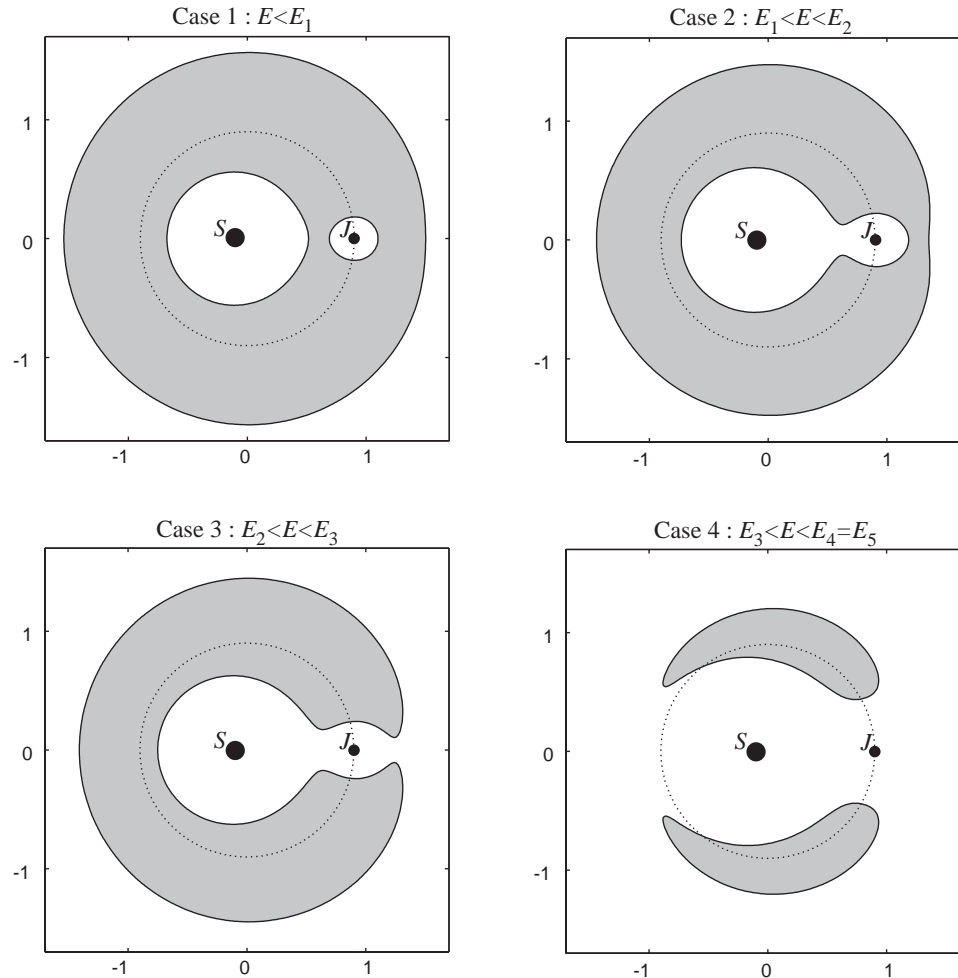
■ *Circular restricted 3-body prob. (2D)*

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



3-Body Problem (2D)

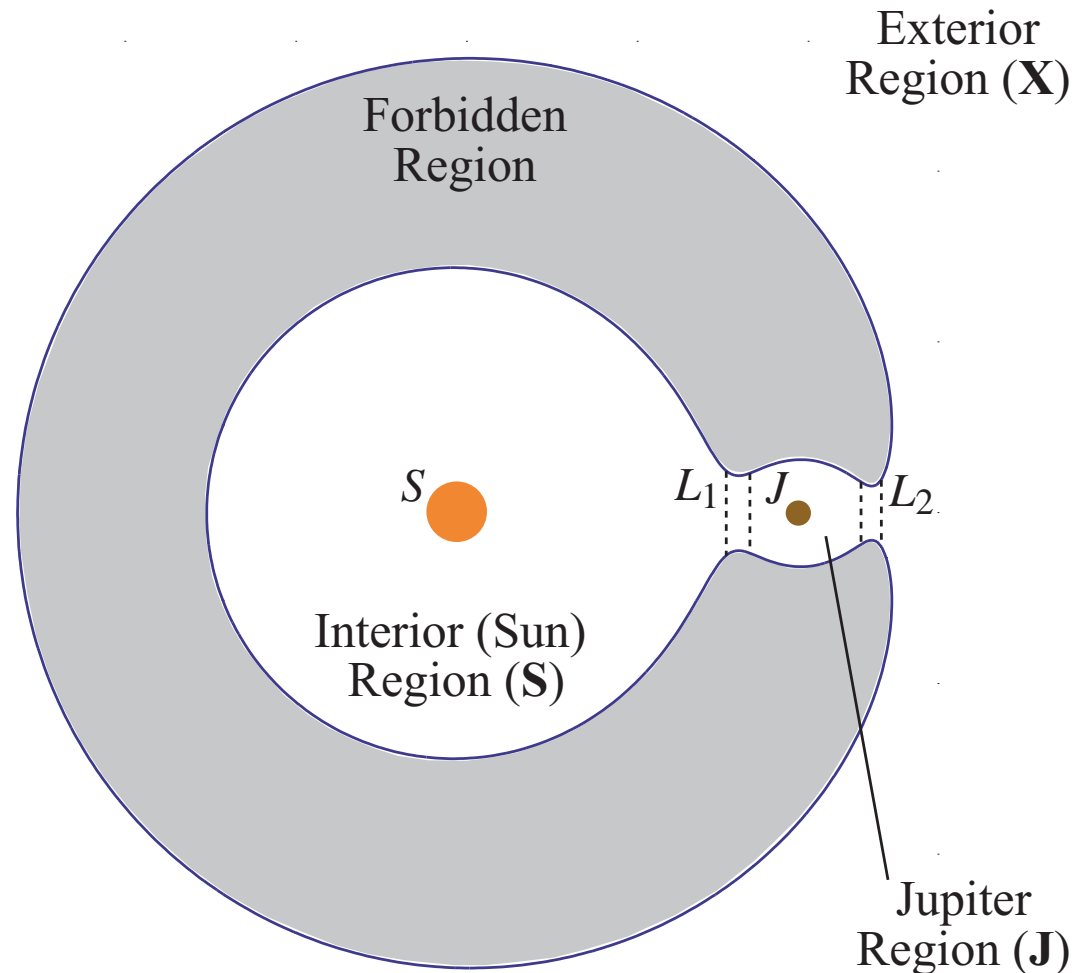
■ *Look at fixed energy*



Position Space Projections

3-Body Problem (2D)

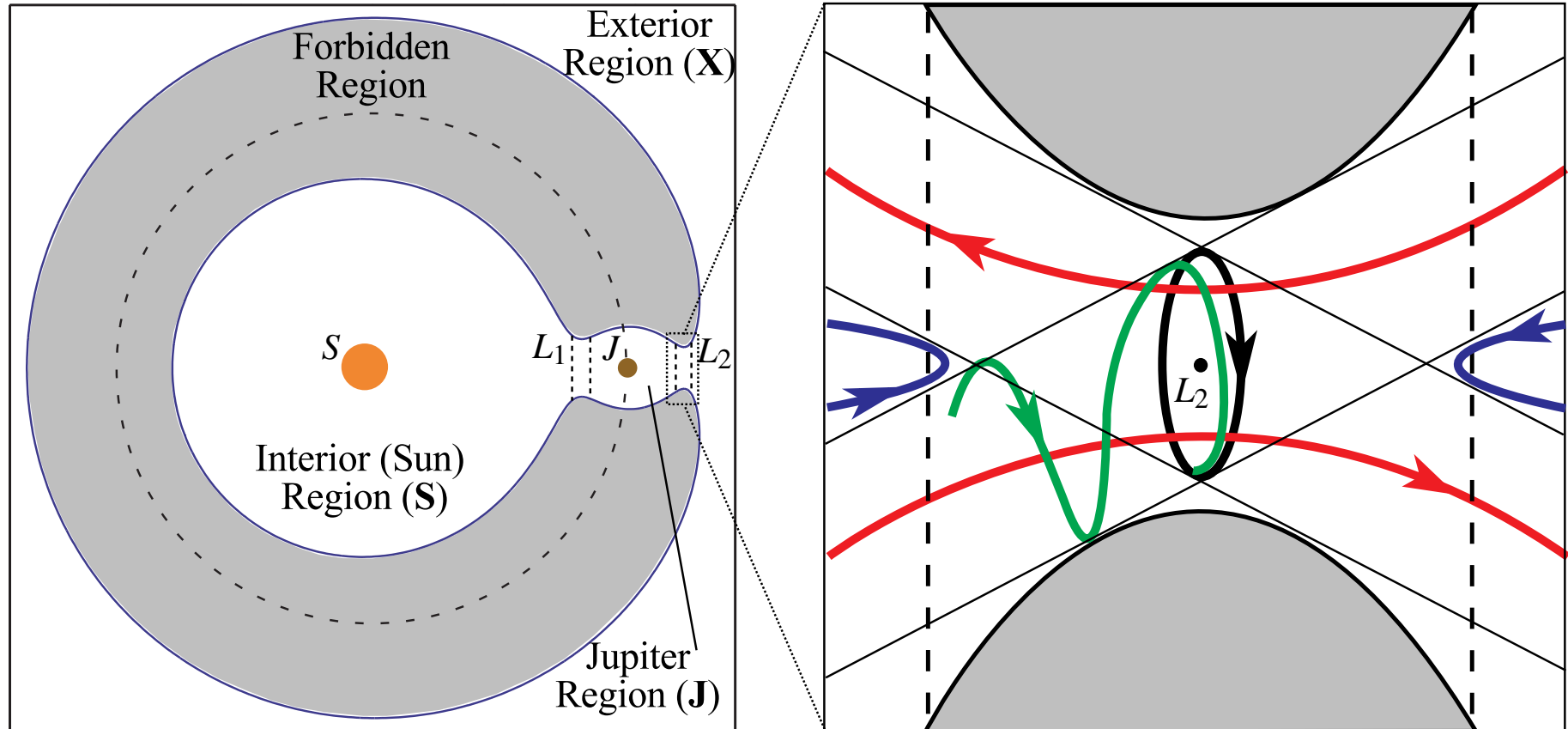
■ *Partition the energy surface*



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

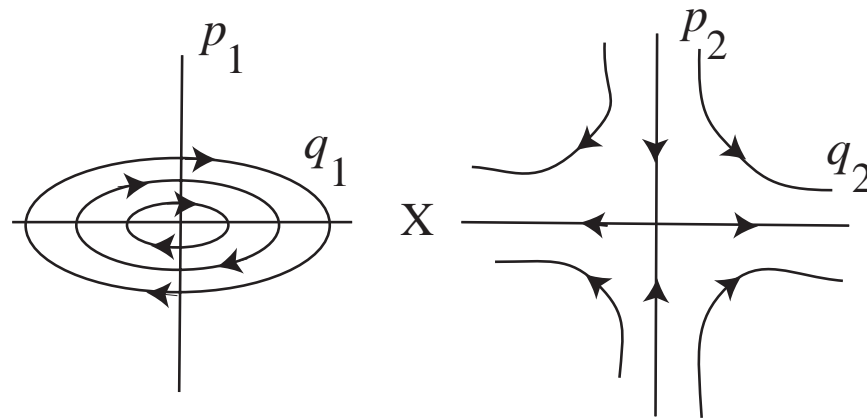
$$H(q, p) = \frac{\omega}{2}(q_1^2 + p_1^2) + \lambda q_2 p_2, \quad (1)$$

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.,

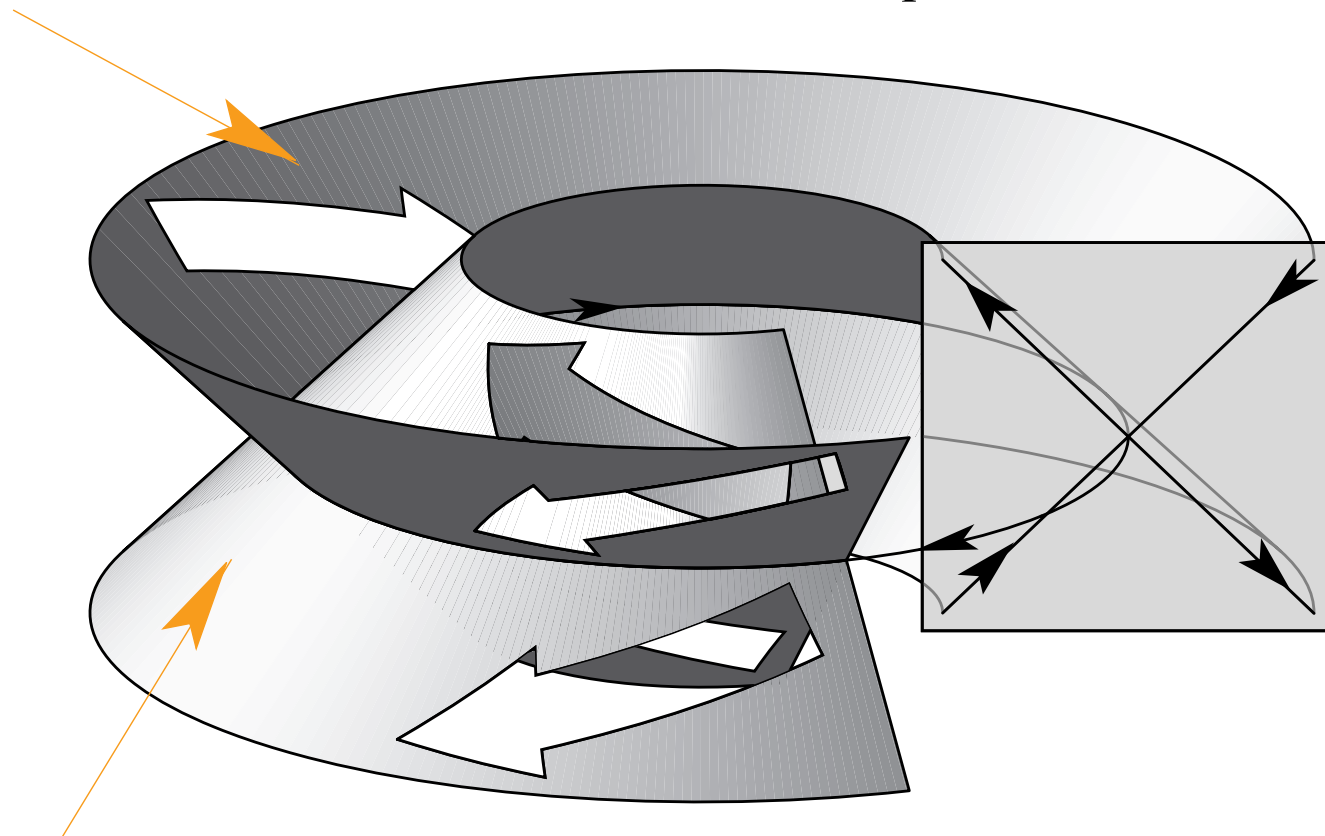
$$\mathcal{M}_h = \frac{\omega}{2}(q_1^2 + p_1^2) = h > 0.$$

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

Local Dynamics

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

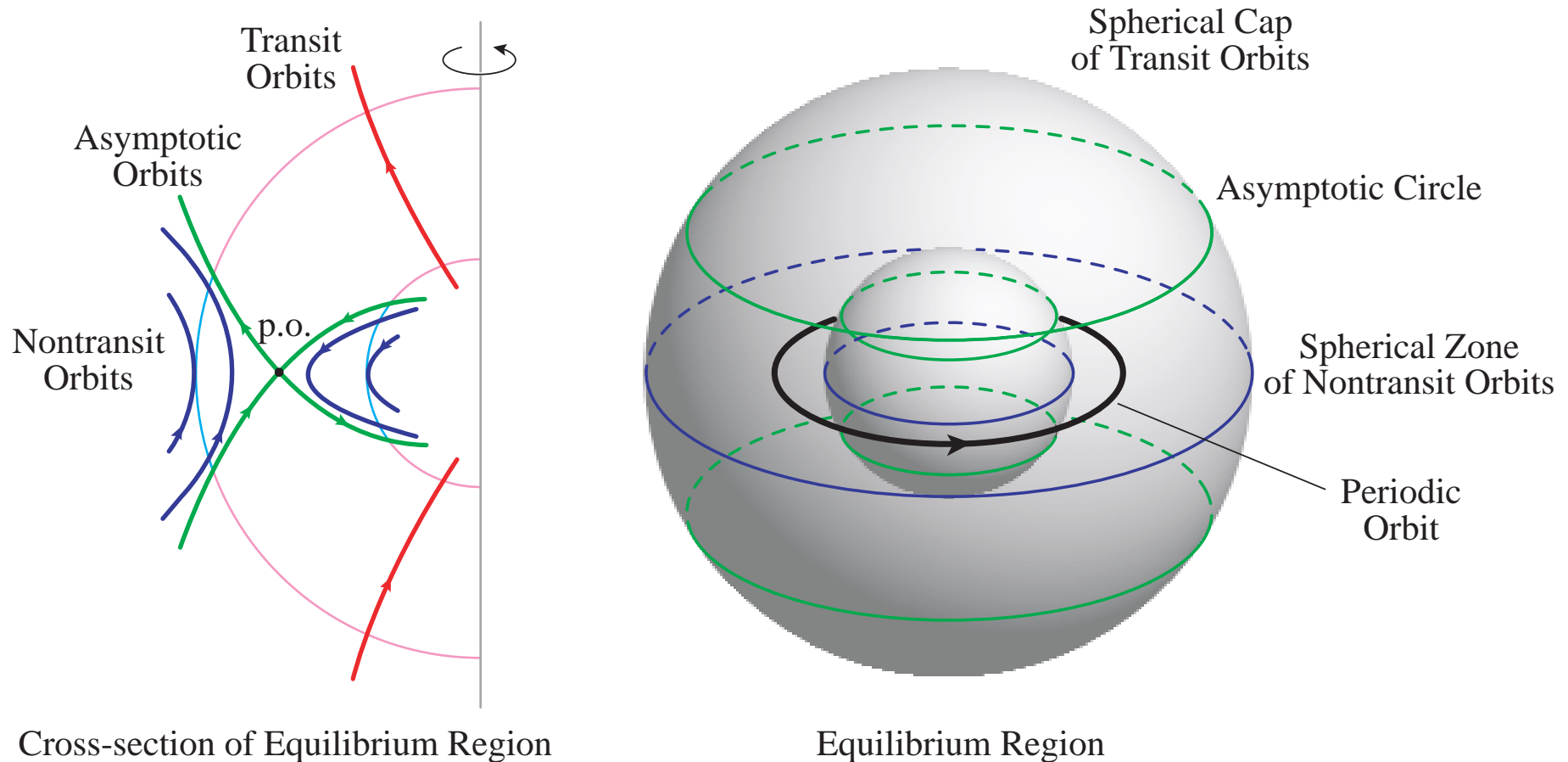
Stable Manifold (orbits move toward the periodic orbit)



Unstable Manifold (orbits move away from the periodic orbit)

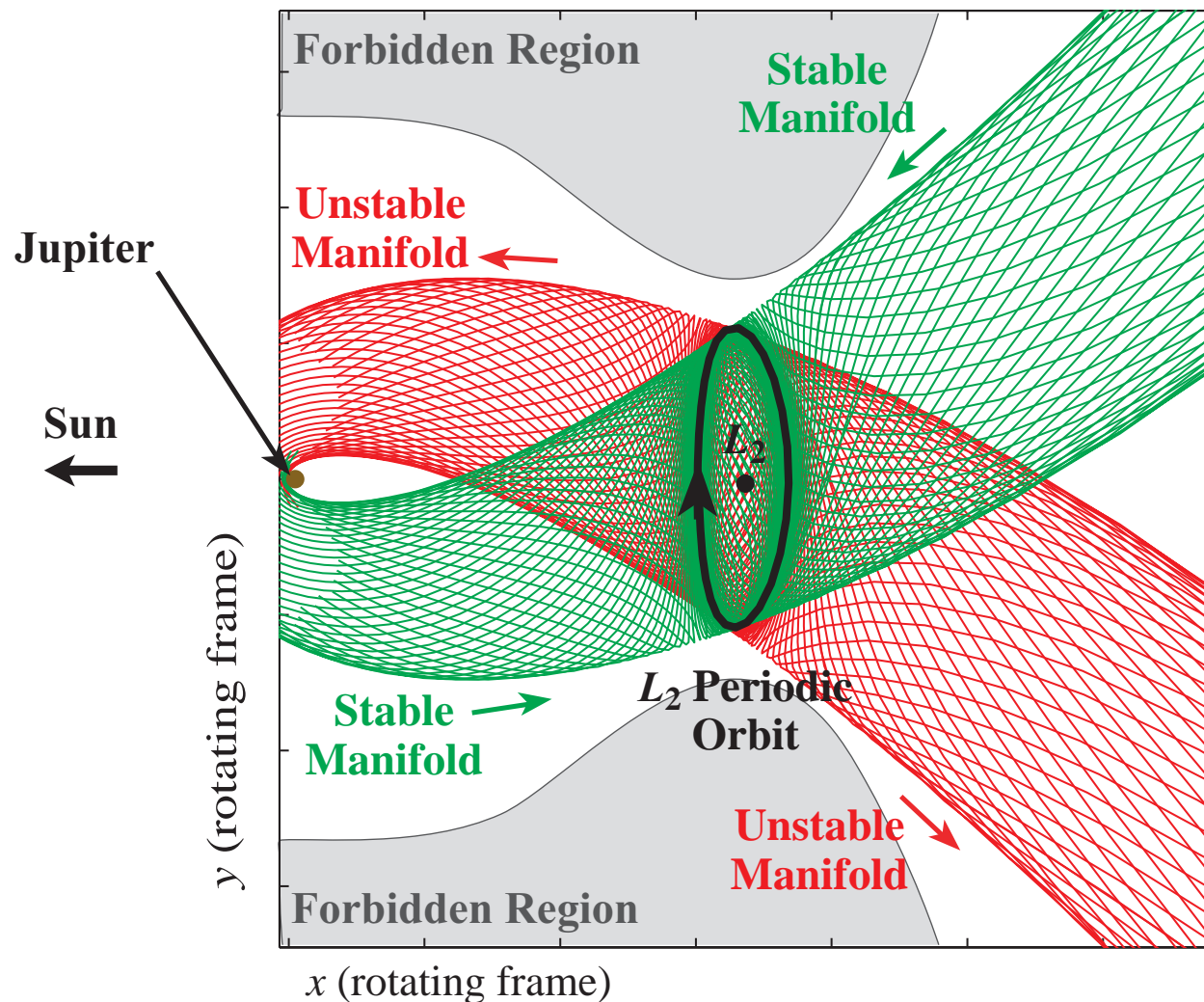
Transit and Nontransit Orbits

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



Tubes in the 3-Body Problem

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

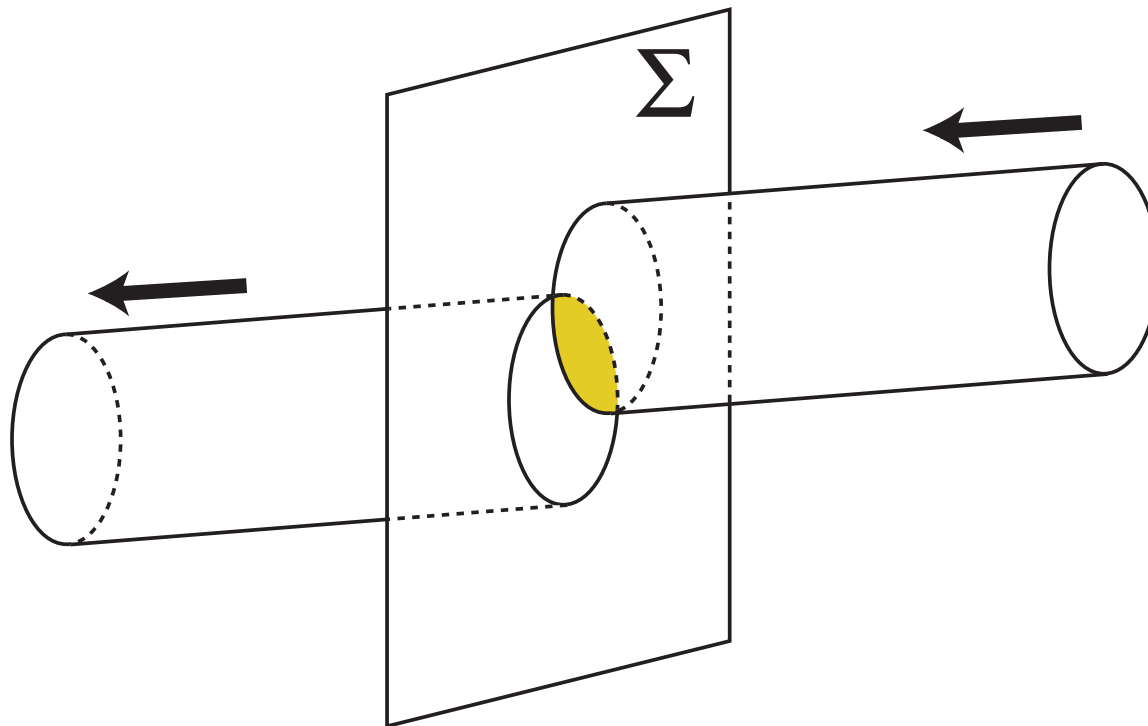


Flux

- *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 Probabilities

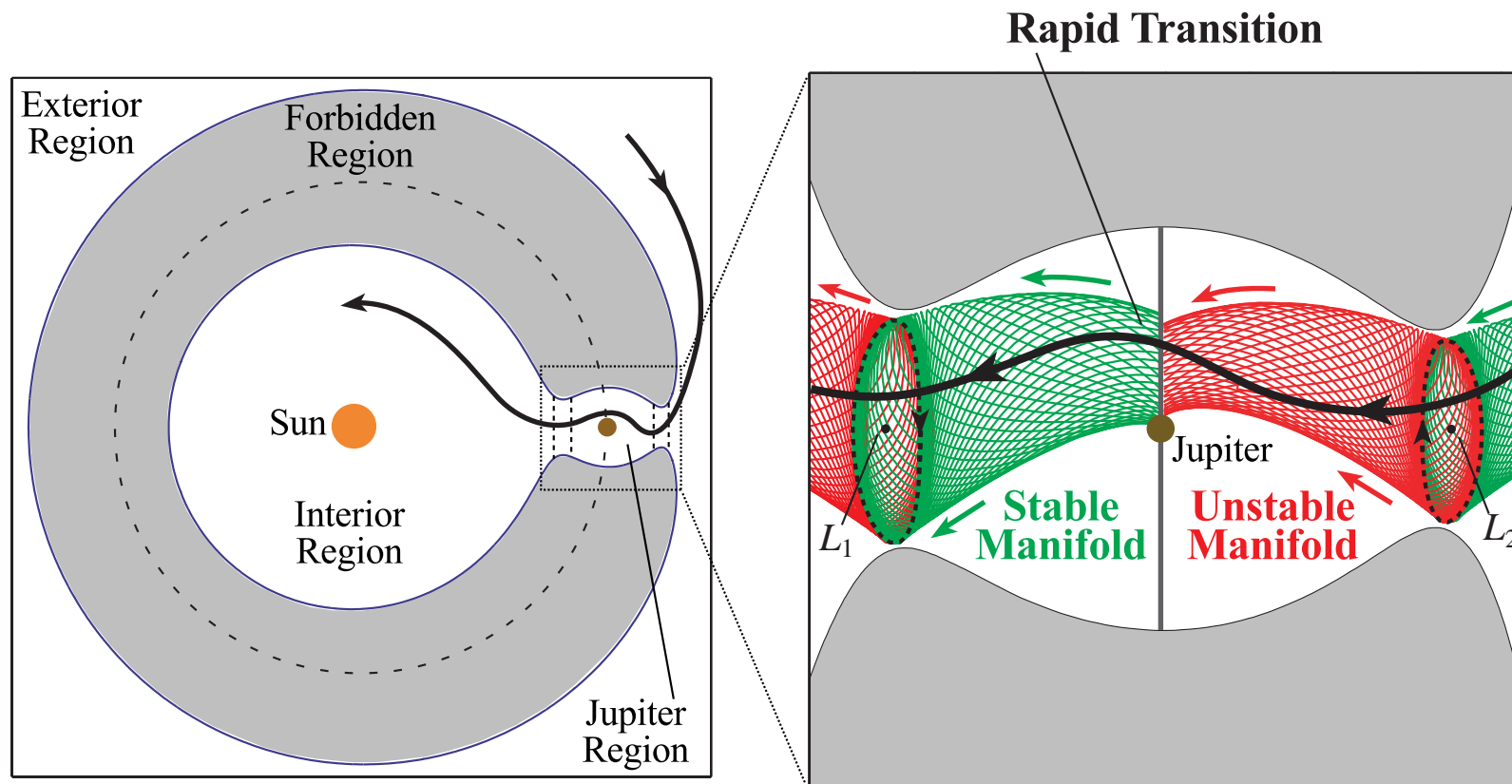
- *More exotic transport between regions*
 - Look at the intersections between the interior of stable and unstable tubes on the same energy surface.
 - Could be from different potential barrier saddles.



Poincaré Section

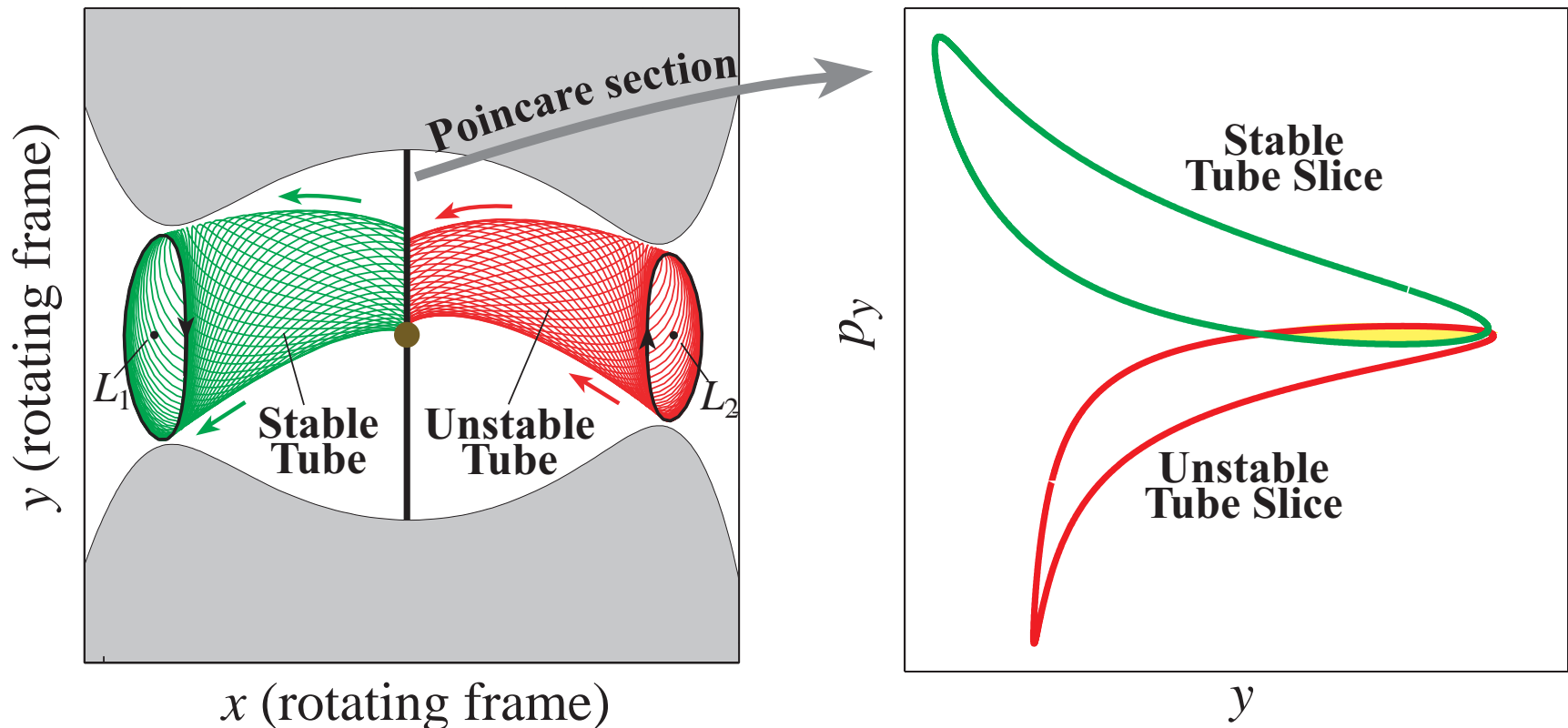
Transition Probabilities

- Example: Comet transport between outside and inside of Jupiter



Transition Probabilities

- 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) .

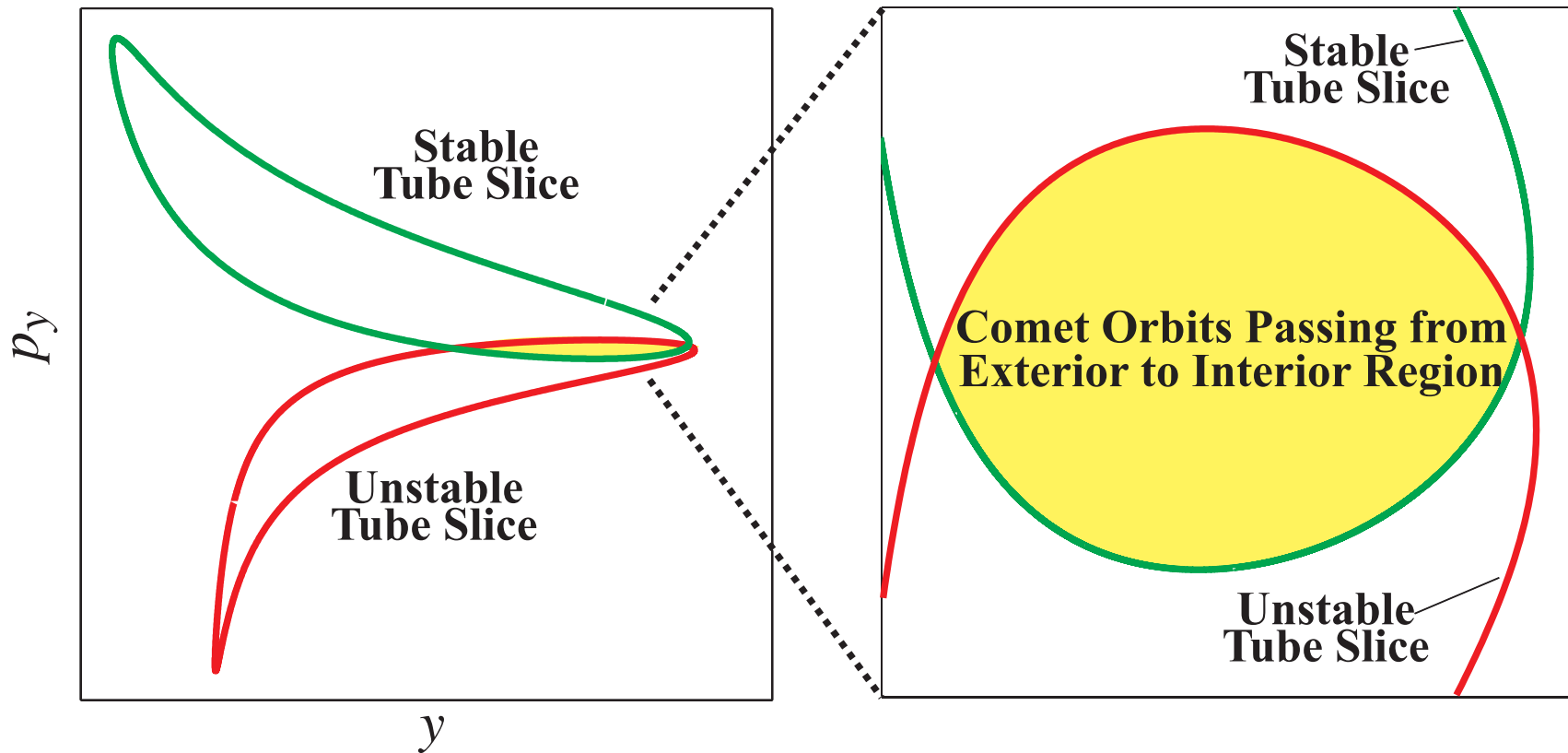


Position Space

Canonical Plane (y, p_y)

Transition Probabilities

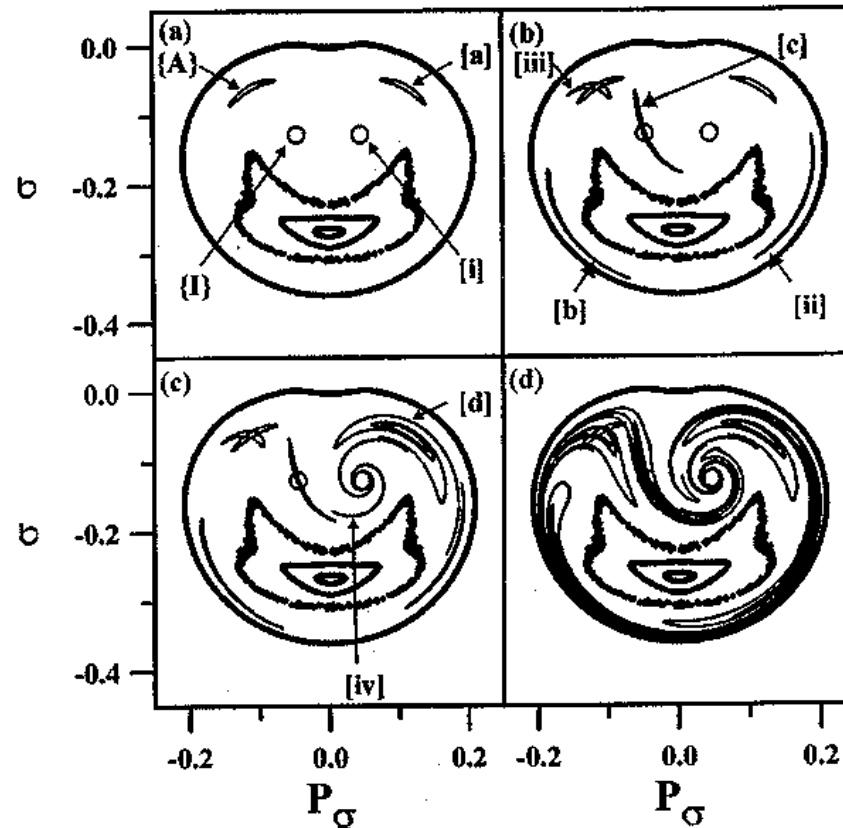
- Relative canonical area gives relative volume of orbits.
- Under certain ergodic assumptions, the relative volume can be interpreted as the probability of transition.



Canonical Plane (y, p_y)

Mixing

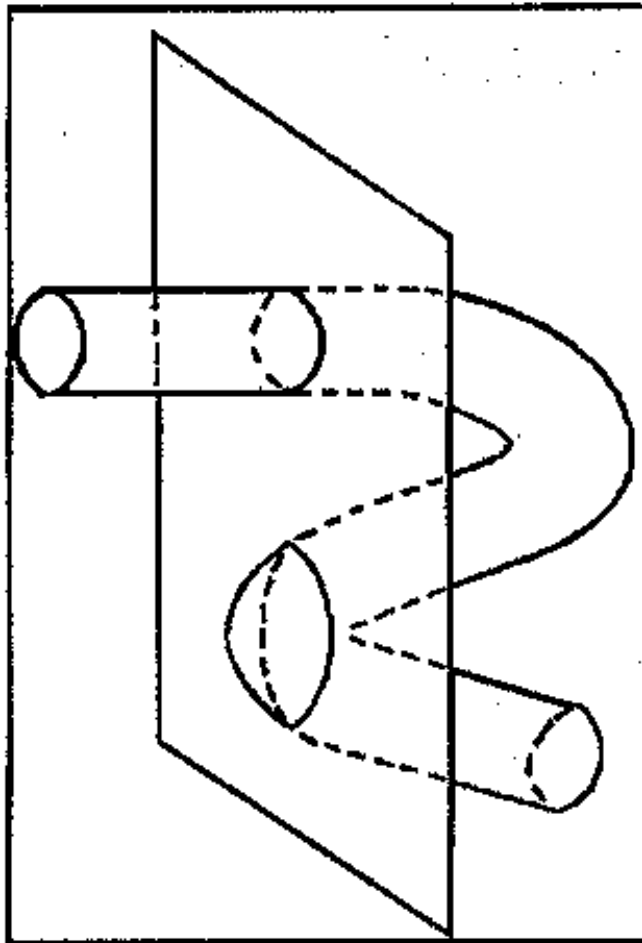
- By keeping track of the intersections of the tubes, one can describe the mixing of different regions ($T_{i,j}(t)$).
 - It can get messy fast!



(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 $\pm i\omega_j$, $j = 1, \dots, N - 1$, and $\pm\lambda$.
- Assume the complexification is diagonalizable.
- Hamiltonian normal form theory transforms Hamiltonian into a lowest order form:
$$H(q, p) = \sum_{i=1}^{N-1} \frac{\omega_i}{2} (p_i^2 + q_i^2) + \lambda q_N p_N.$$
- Equilibrium point is of type center $\times \dots \times$ center \times saddle ($N - 1$ centers).

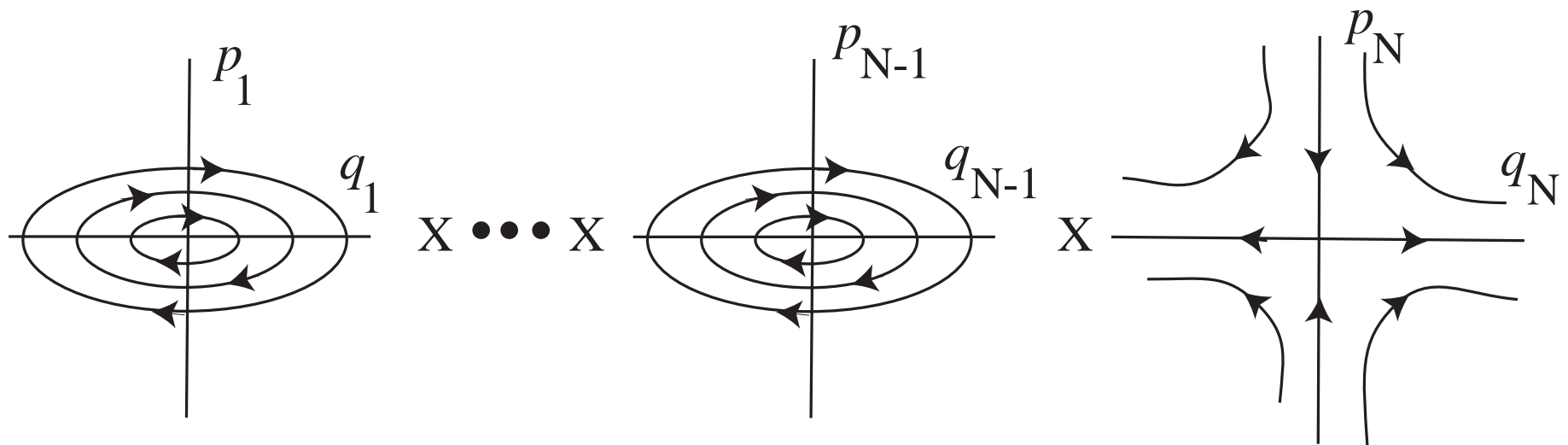
$N = 3$ or More

■ *Multidimensional “saddle point”*

□ For fixed energy $H = h$, energy surface $\simeq S^{2N-2} \times \mathbb{R}$.

□ Constants of motion:

$$I_j = q_j^2 + p_j^2, j = 1, \dots, N - 1, \text{ and } I_N = q_N p_N.$$



The N Canonical Planes

$N = 3$ or More

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

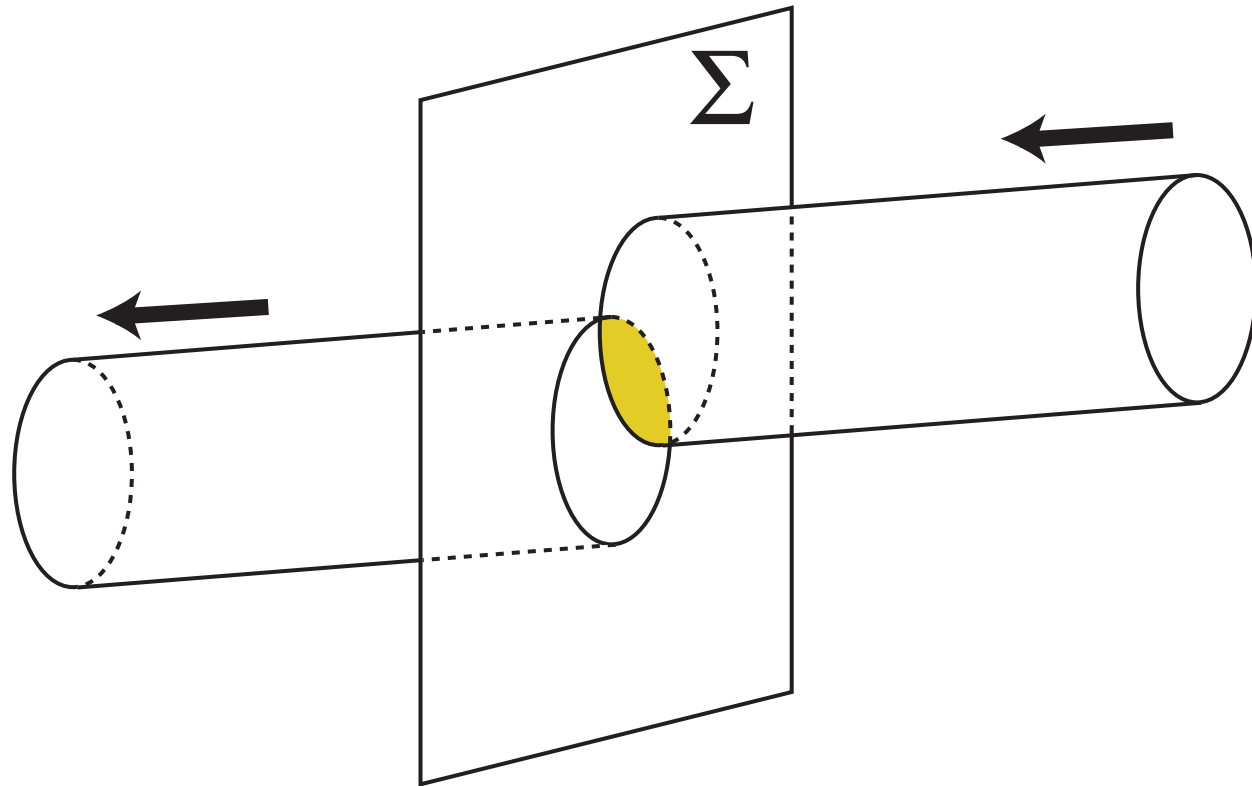
$$\mathcal{M}_h = \sum_{i=1}^{n-1} \frac{\omega_i}{2} (p_i^2 + q_i^2) = h > 0.$$

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

- Four “cylinders” of asymptotic orbits: the stable and unstable manifolds $W_{\pm}^s(\mathcal{M}_h), W_{\pm}^u(\mathcal{M}_h)$, which have the structure $S^{2N-3} \times \mathbb{R}$.

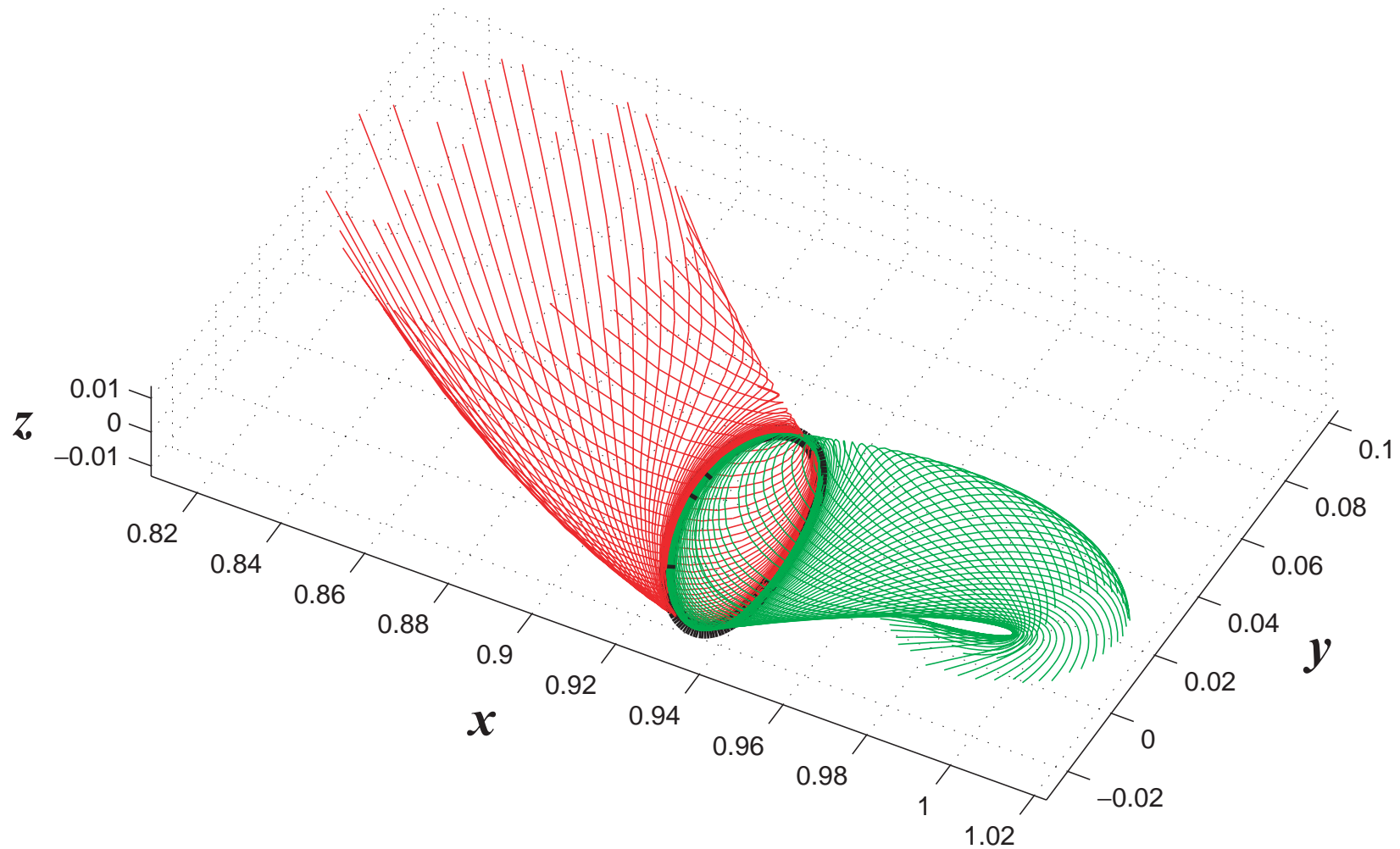
$N = 3$ or More

- 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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