Global Analysis w/ Invariant Manifold Tube Transport

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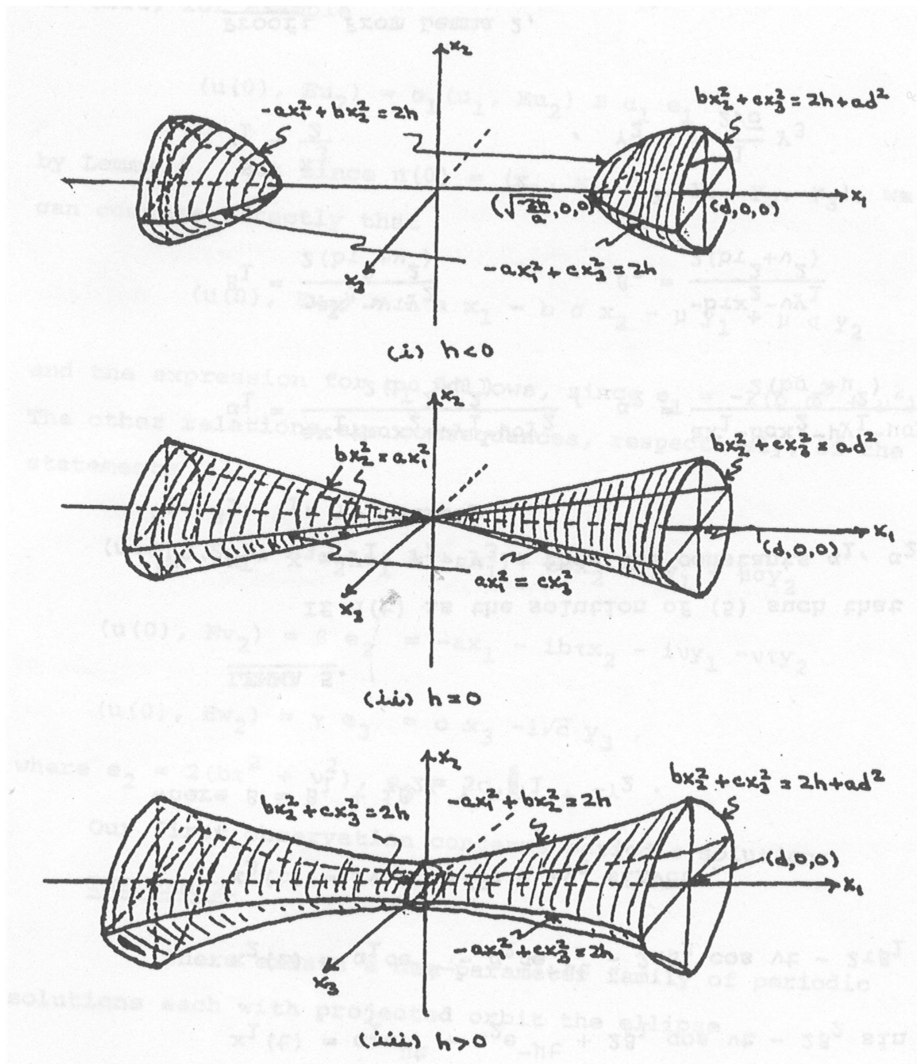
Organization of Talk

- Theory of Invariant Manifold Tubes
  - **Restricted Three Body Problem (R3BP)**
- Computational Methods
  - **High order normal form expansions**
  - **Monte Carlo sampling of energy surface**
- Chemical Reaction Dynamics
  - **Electron scattering in the Rydberg atom**
  - **Planar scattering of H_2O with H_2**

A Historical Perspective

- **Appleyard [1970]: Invariant sets near unstable Lagrange points of R3BP.**
  - First picture of transport tube.



Invariant Manifold Tubes

- What are tubes and where do they live?
  - **Geometry**
- What do tubes do (prediction/control)?
  - **Dynamics**

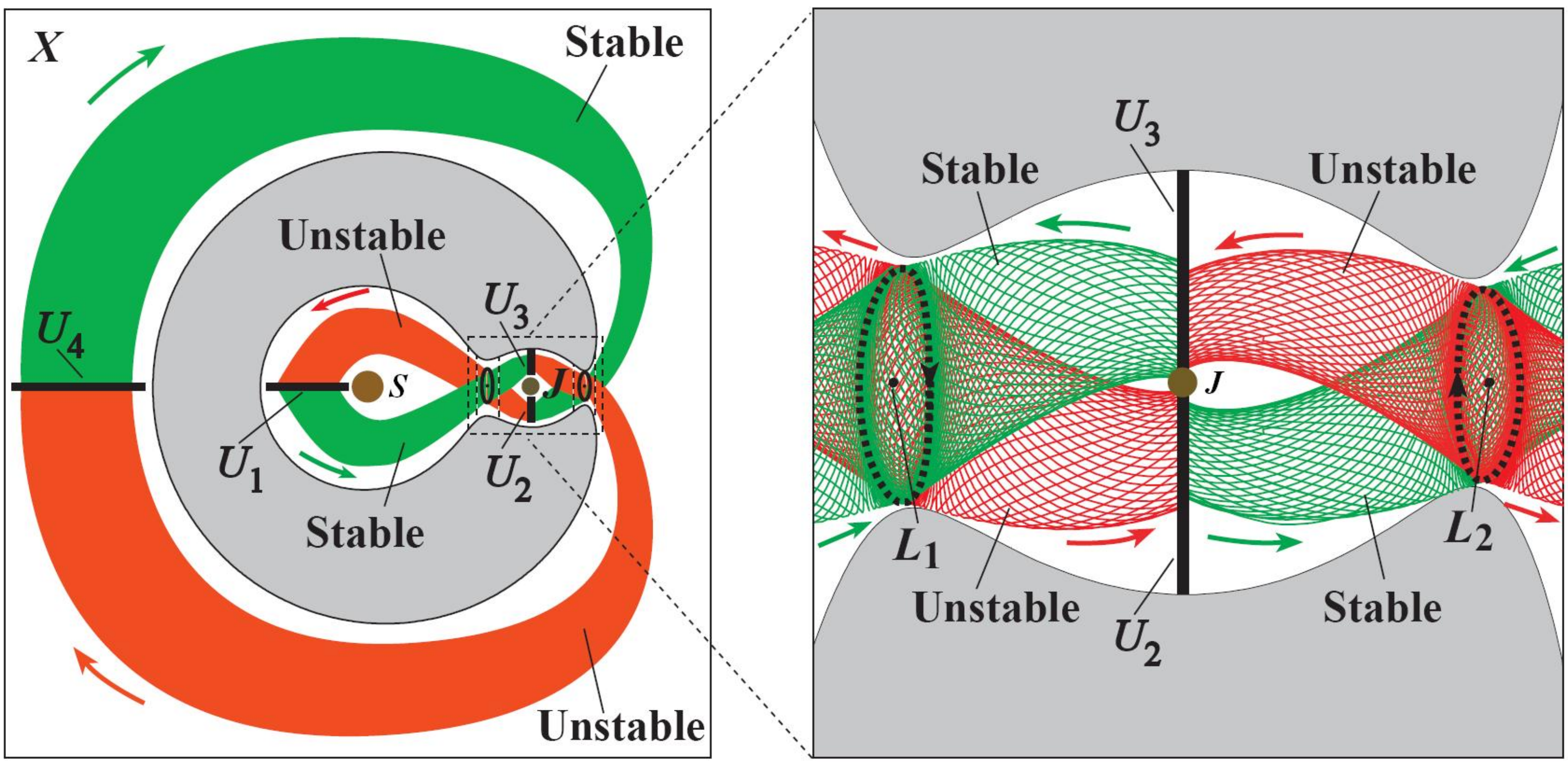
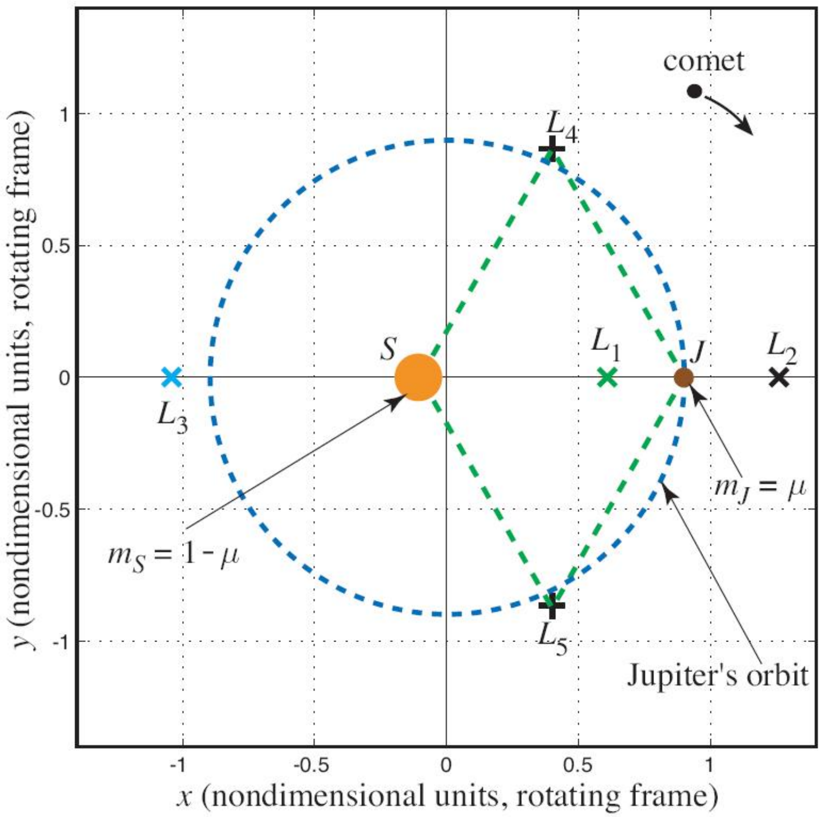
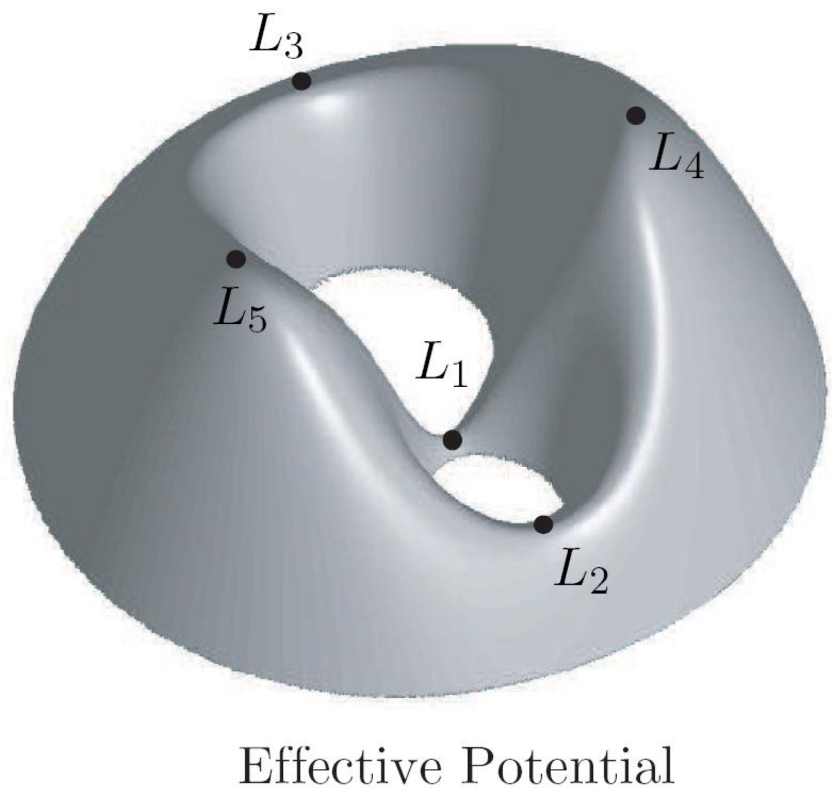


Figure from Gomez, Koon, Lo, Marsden, Masdemont, & Ross 2001

Restricted Three Body Problem





Figures from Marsden and Ross 2006

- Left: Fixed points viewed in rotating frame
- Right: Hill's Region (potential energy surface)

Low Energy Saddle Points

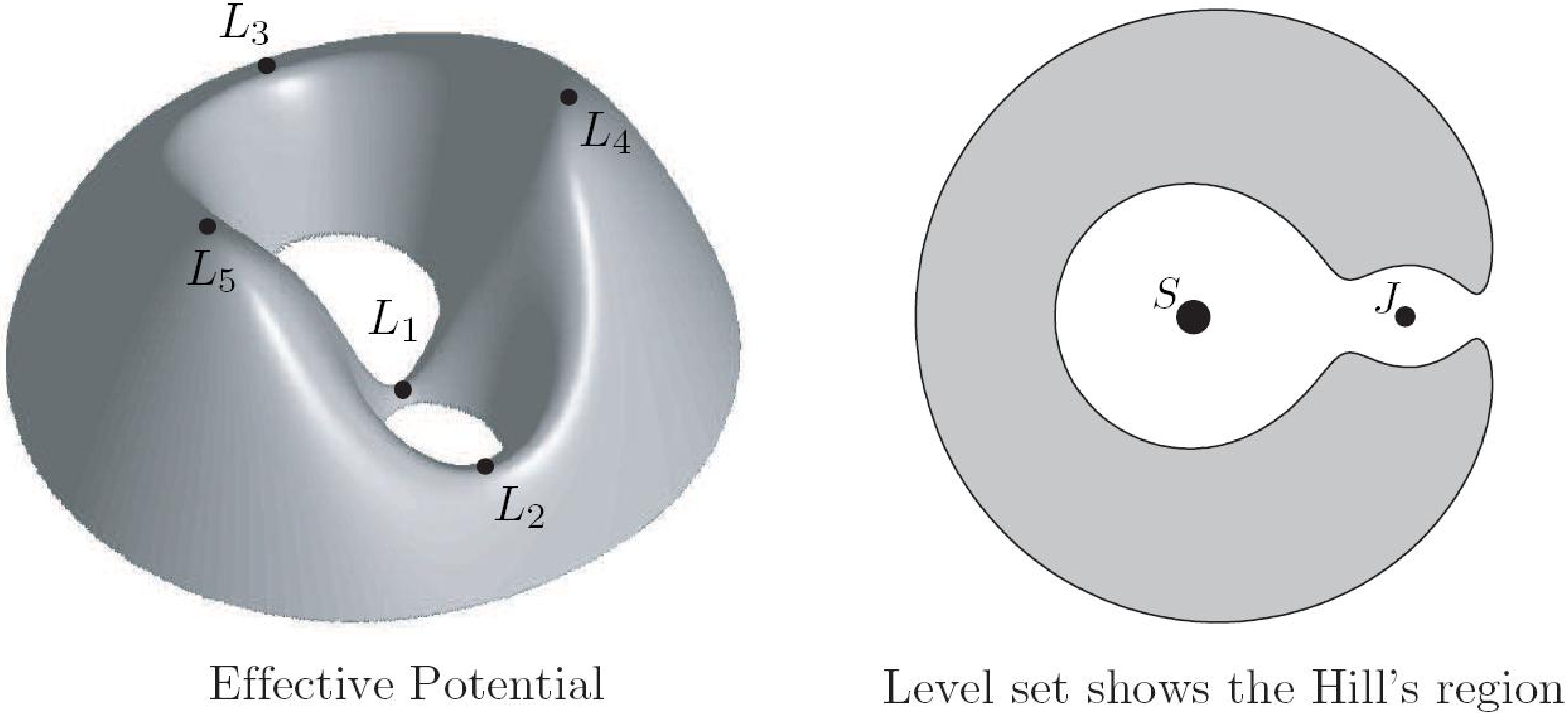


Figure from Koon, Lo, Marsden, & Ross 2000

- Reduce out rotations and work at fixed ang. mom.
- L_1 & L_2 are low energy saddle points
  - **mediate transport from inner and outer realms**

$L_{1,2,3}$ are Rank-1 Saddles

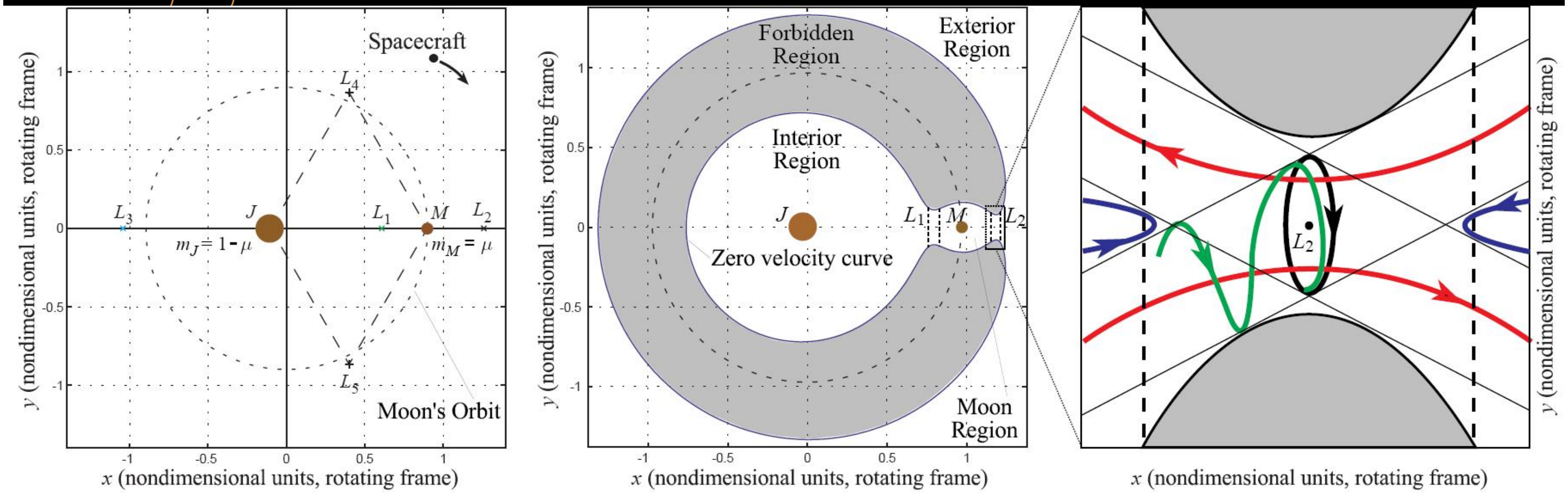


Figure from Koon, Lo, Marsden & Ross 1999a

$$H_2 = \lambda q_1 p_1 + \frac{1}{2}\omega_1\left(q_2^2 + p_2^2\right) + \frac{1}{2}\omega_2\left(q_3^2 + p_3^2\right)$$

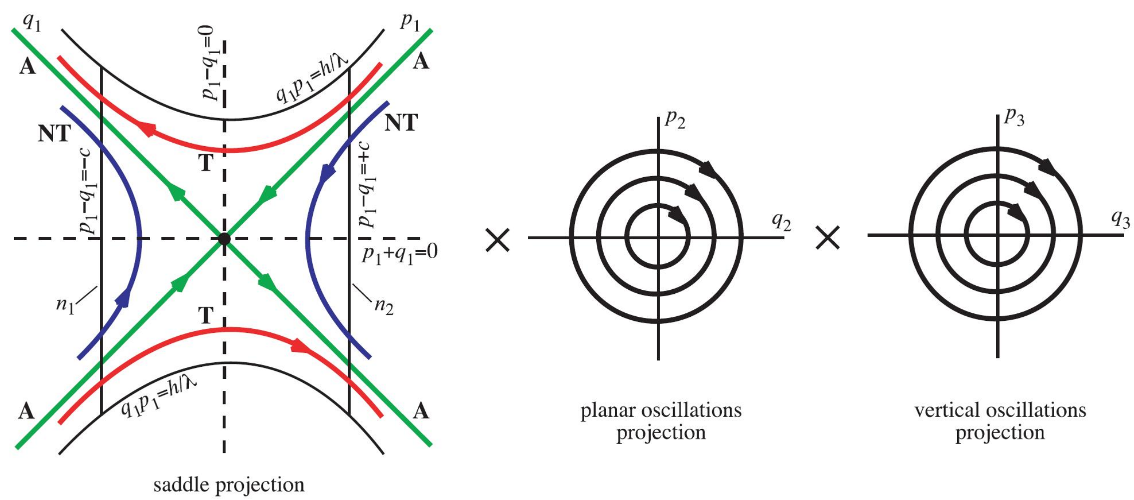


Figure from Gomez, Koon, Lo, Marsden, Masdemont, & Ross 2001

Rank-1 Saddle Geometry

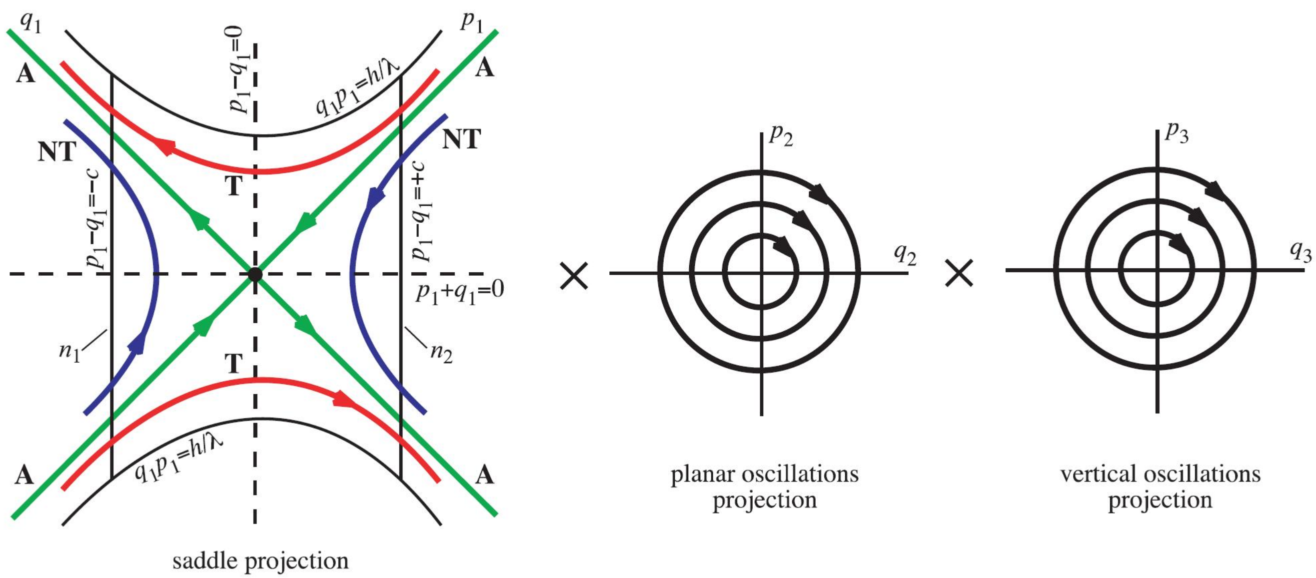
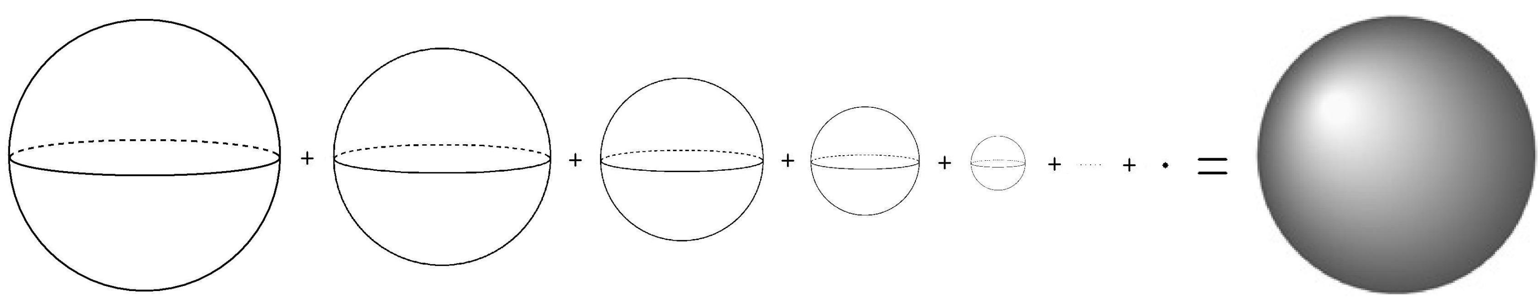


Figure from Gomez, Koon, Lo, Marsden, Masdemont, & Ross 2001

- Energy is shared between saddle and two centers

$$S^3 \cong \left\{ \frac{\omega_1}{2}\left(q_2^2 + p_2^2\right) + \frac{\omega_2}{2}\left(q_3^2 + p_3^2\right) = H - \lambda q_1 p_2 \right\}$$



Orbit Structures

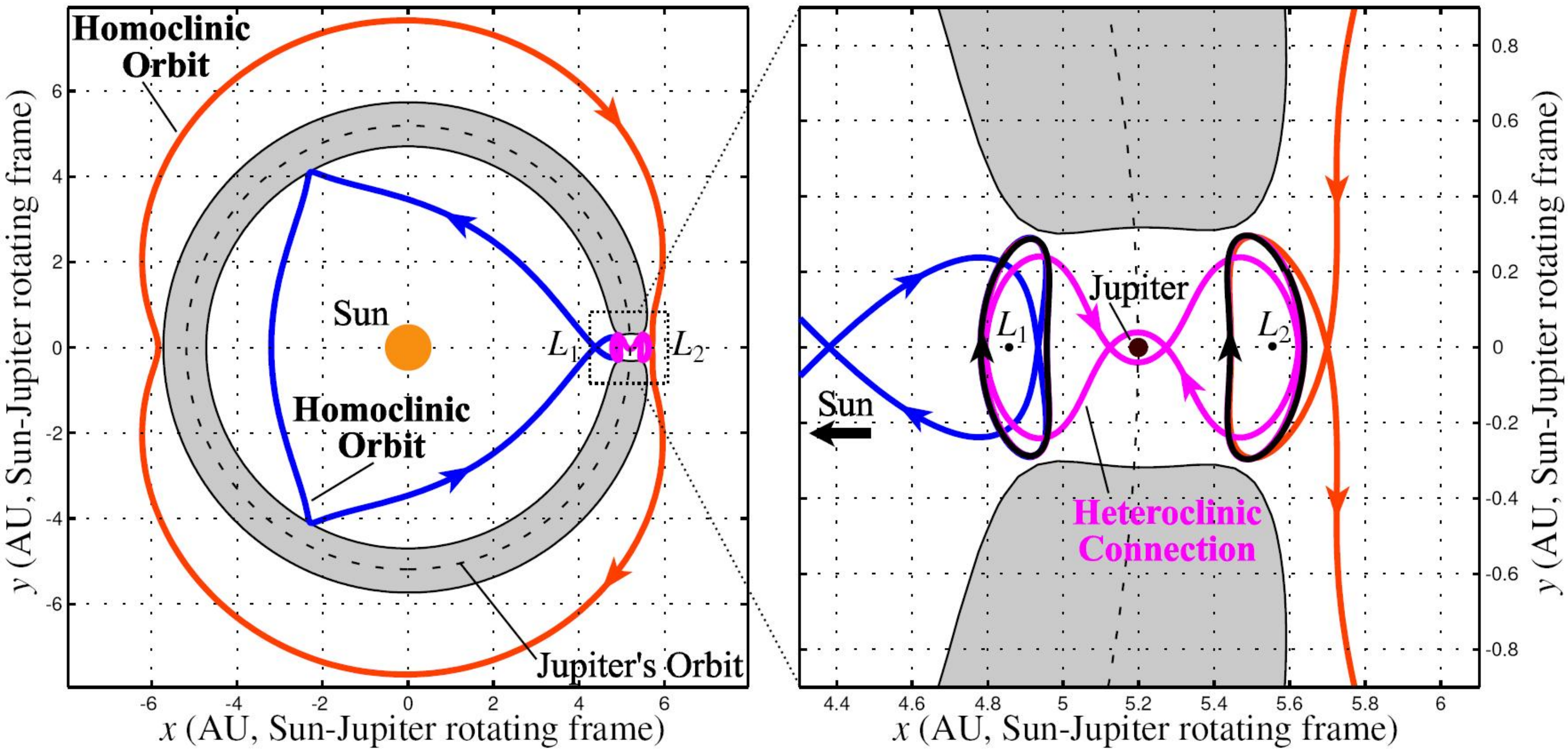


Figure from Koon, Lo, Marsden, & Ross 1999b

- Conley [1968]: Low energy transit orbits
- McGehee [1969]: Homoclinic orbits

Symbolic Dynamics

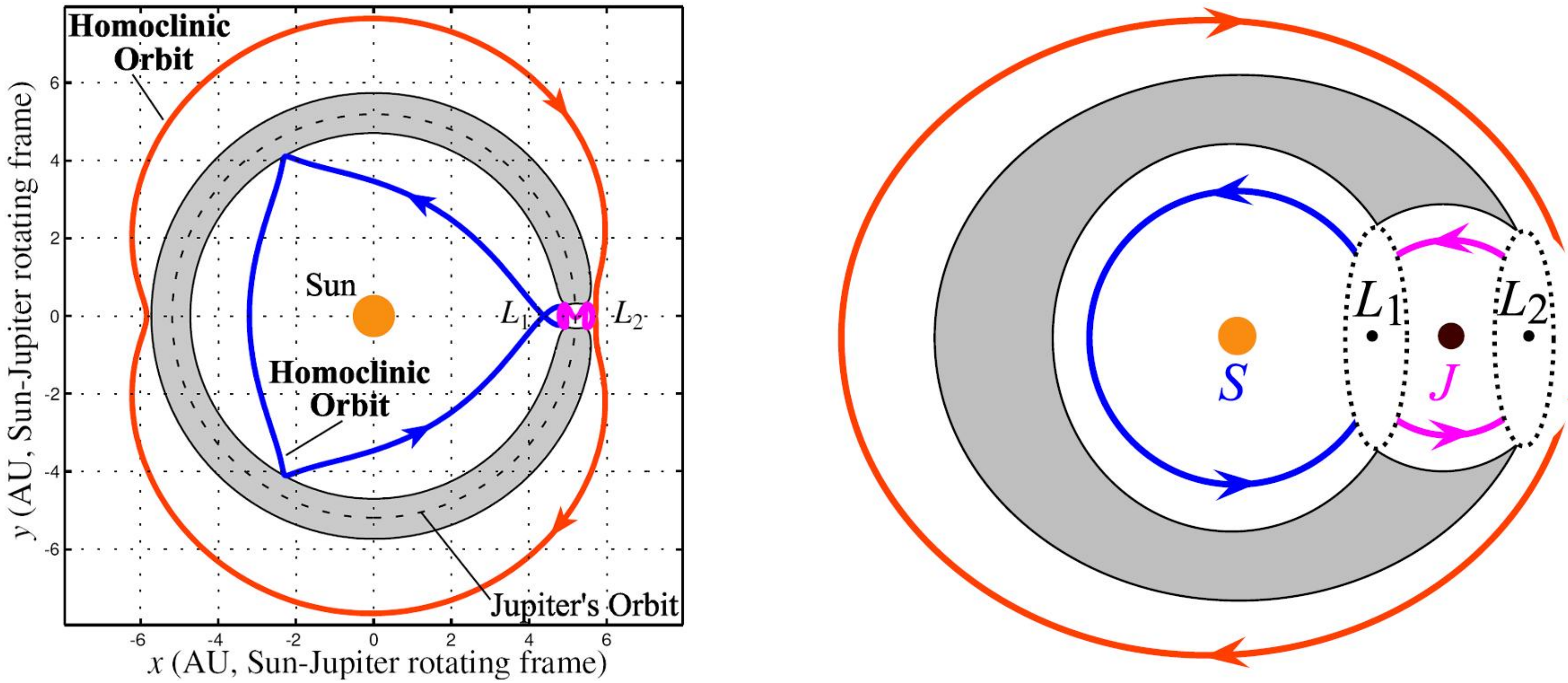


Figure from Koon, Lo, Marsden, & Ross 1999b

- Symbolic/horseshoe dynamics
- **Thm.** [Koon, Lo, Marsden, Ross, *Chaos* 2000]:
  - **There is an orbit with any admissible itinerary**
  - **Example:** $(\ldots,\mathbf{X},\mathbf{J},\mathbf{S},\mathbf{J},\mathbf{X},\ldots)$

Manifold Tube Intersections

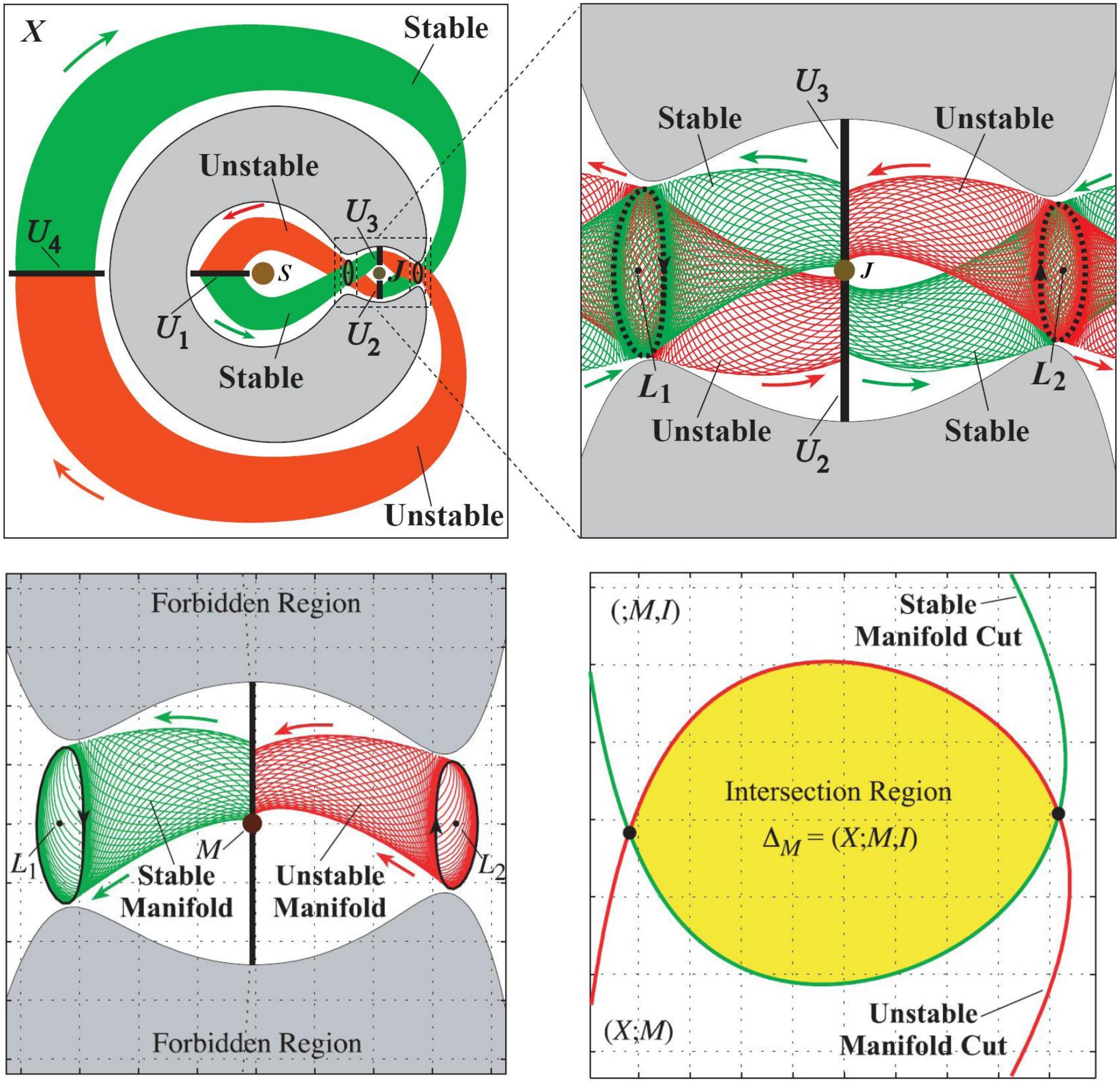


Figure from Gomez, Koon, Lo, Marsden, Masdemont, & Ross 2001

Patched Three Body Problem

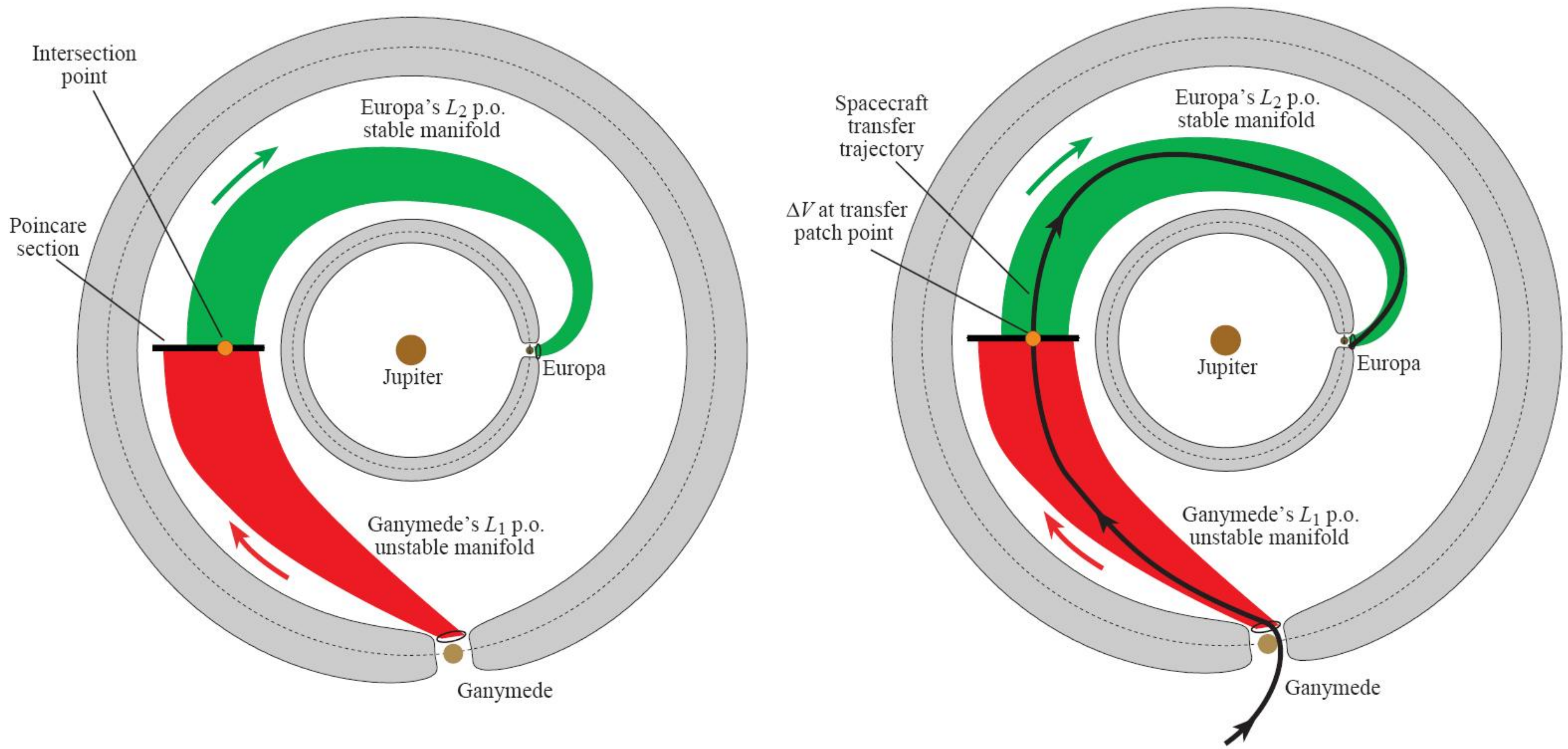


Figure from Gomez, Koon, Lo, Marsden, Masdemont, & Ross 2001

- Jupiter Icy Moons Orbiter (JIMO)
- Arbitrarily many flyby's of each moon

Normal Forms

- Integrable approximation to chaotic dynamics
- Linearize Vector Field at fixed pt.
  - $\dot{z} = D\mathbb{J}\nabla H(z) = Az;\qquad z = (q, p)$
  - **Matrix A has eigenvalues $\pm\lambda, \pm i\omega_1, \pm i\omega_2, \ldots, \pm i\omega_n$**
    - $\pm i\omega_k$ corresponds to elliptic motion (center)
    - $\pm\lambda$ corresponds to hyperbolic motion (saddle)
  - **Transport is governed by $\pm\lambda$ direction**
- NF decouples saddle & center modes to high order

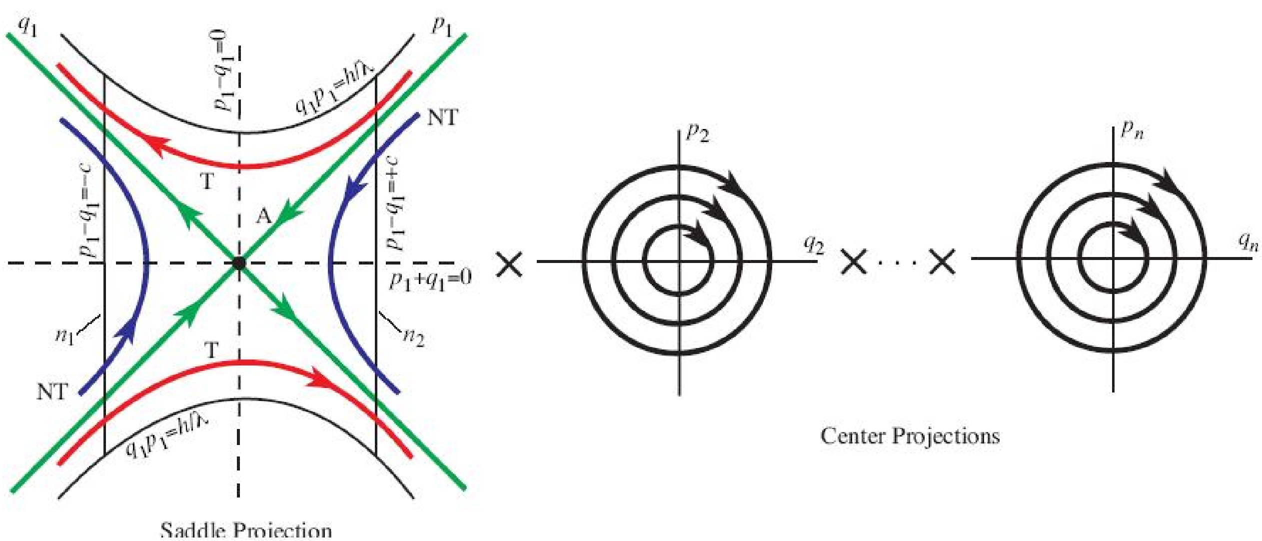


Figure from Gomez, Koon, Lo, Marsden, Masdemont, & Ross 2001

Normal Form at Rank-1 Saddle

- Quadratic Normal Form:

$$H_2 = \lambda q_1 p_1 + i\frac{\omega_1}{2}(q_2^2 + p_2^2) + i\frac{\omega_2}{2}(q_3^2 + p_3^2)$$

- Successive transformations eliminate n^{th} order terms
  - **Computations use Lie Transform method:**

    $$\hat{H} = H + \{H, G\} + \frac{1}{2!}\{\{H, G\}, G\} + \frac{1}{3!}\{\{\{H, G\}, G\}, G\} +$$

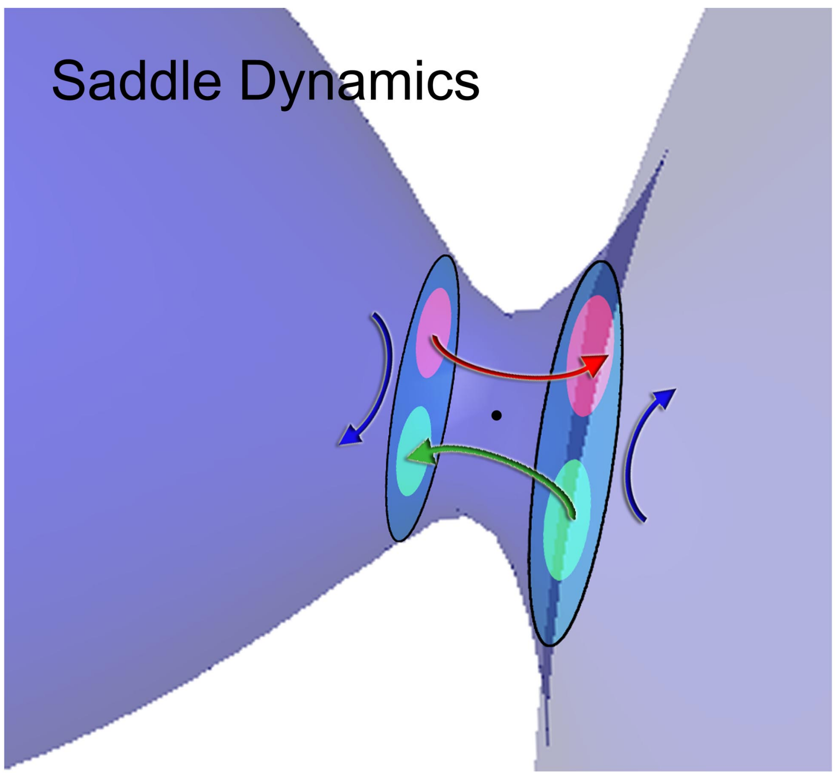
  - **Each change depends only on** A
  - **Kill all terms** $q_1^i p_1^j$ **for** $i \neq j$
- Action-angle variables $(I = q_1 p_1, \theta_k)$
  - $I = 0$ **is reduction to center manifold**
  - $I = \epsilon$ **nudges orbits in saddle direction**
- Implemented for 3DOF systems by A. Jorba (1999)

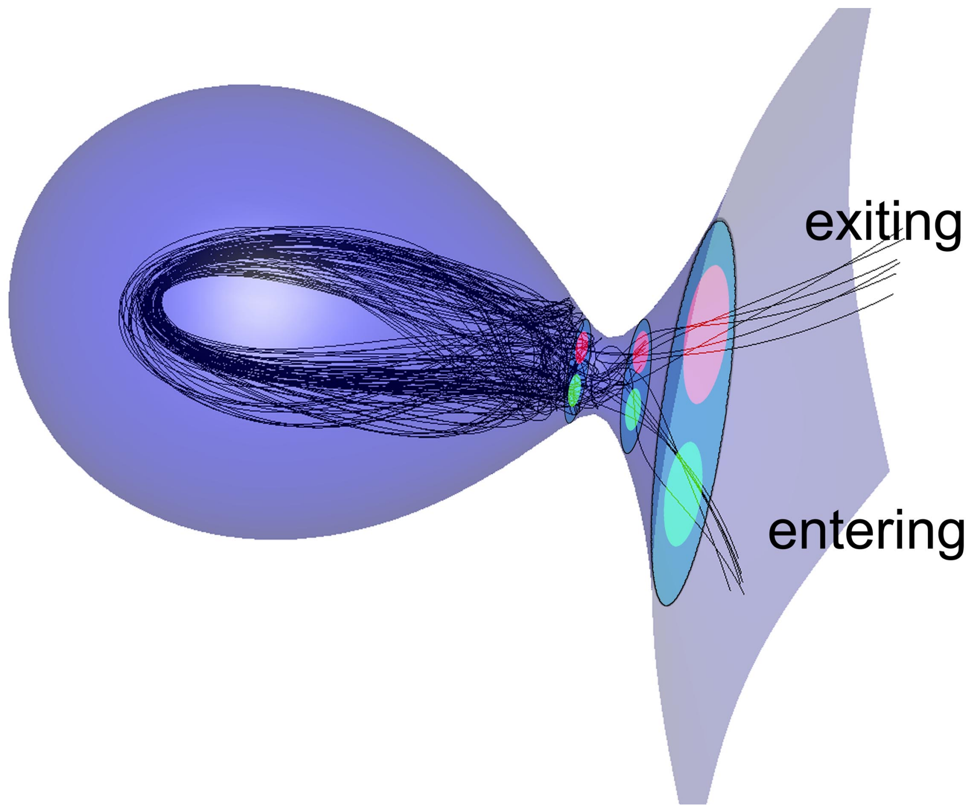
Other Methods

- Global Analysis of Invariant Objects (GAIO)
  - **Transfer operators on box subdivisions**
  - **Tree structured box elimination**
- Statistical Sampling of Trajectories
  - **Monte Carlo sample initial conditions from phase space box surrounding tubes**
  - **Integrate forwards and backwards to determine which tubes the i.c. are in**
  - **After a relatively small number of samples one obtains a good estimate of volume ratios**
  - **Applies well to higher dimensional systems ($\sim$5 or $\sim$10 DOF)**

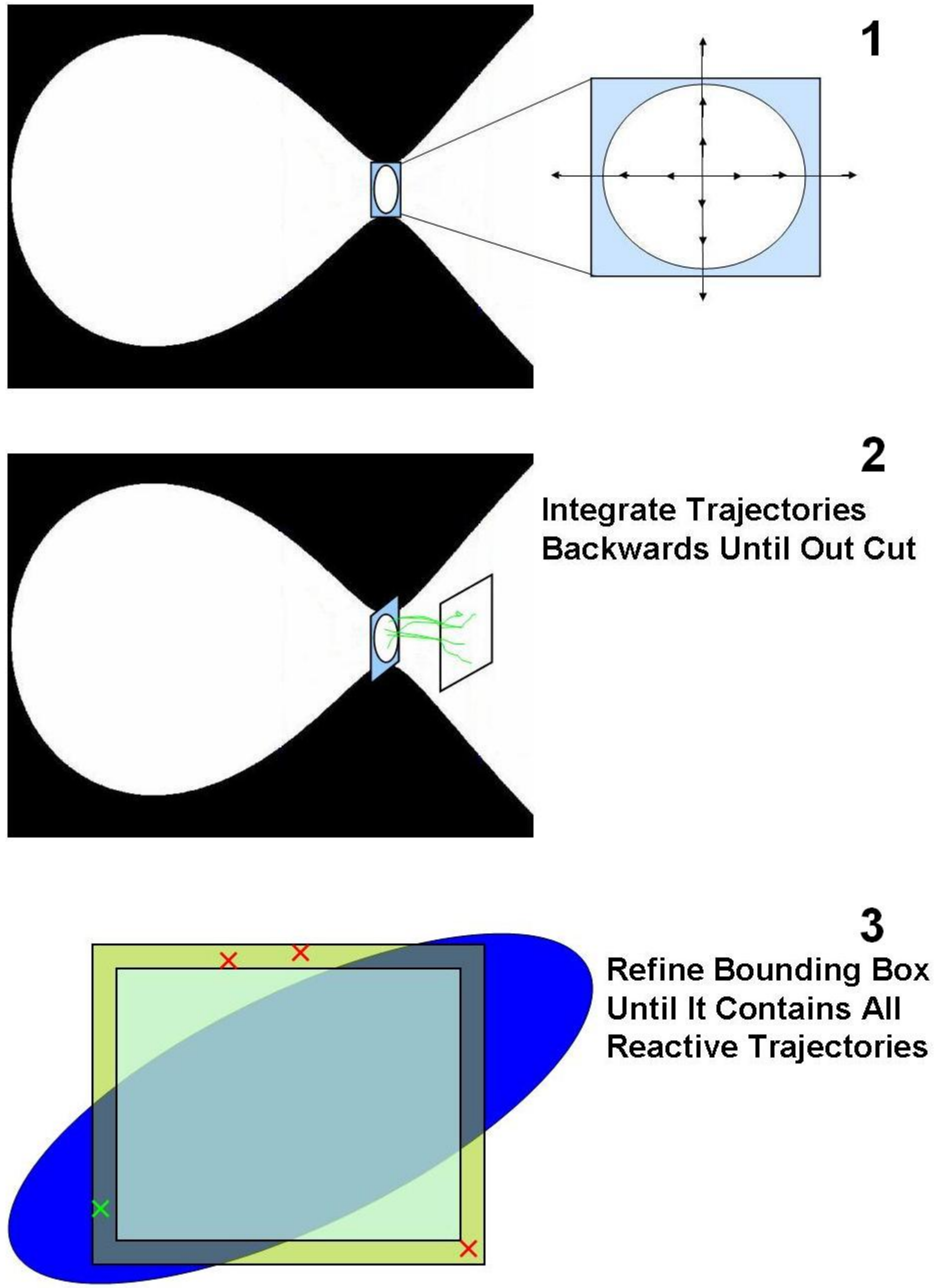
Overview of Method

- ☐ Identify Saddle/TS & Hill Region
- ☐ Find Box Bounding Reactive Trajectories (outcut)
  - **in & out cuts make "airlock"**
  - **Monte Carlo sample energy surface in box**
- ☐ Integrate traj's into bound state until escape



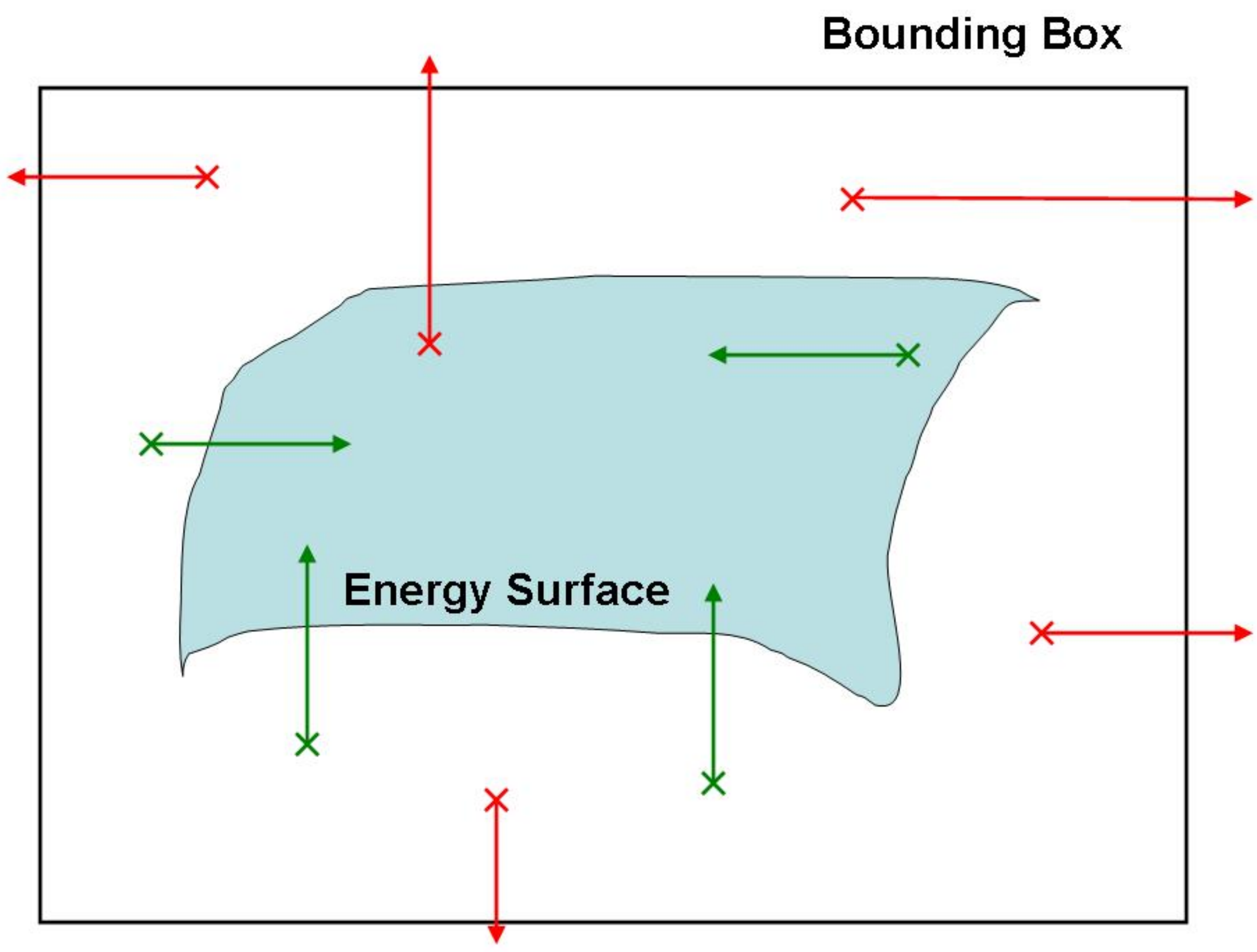


Bounding Box Method

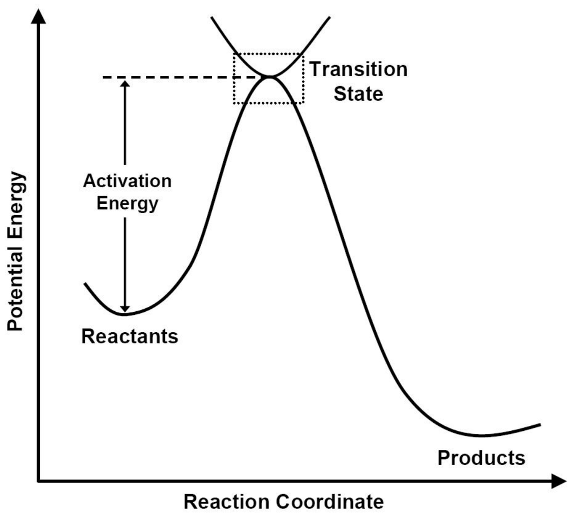


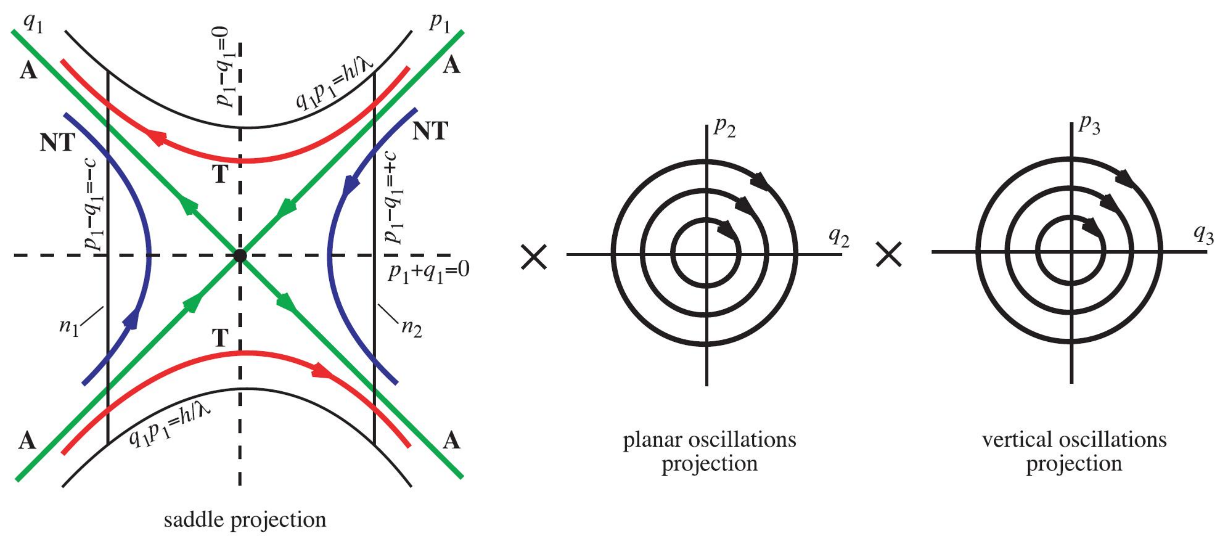
Sampling the Energy Surface

- Randomly select points in bounding box
- Project (using momentum variables) until intersects energy surface



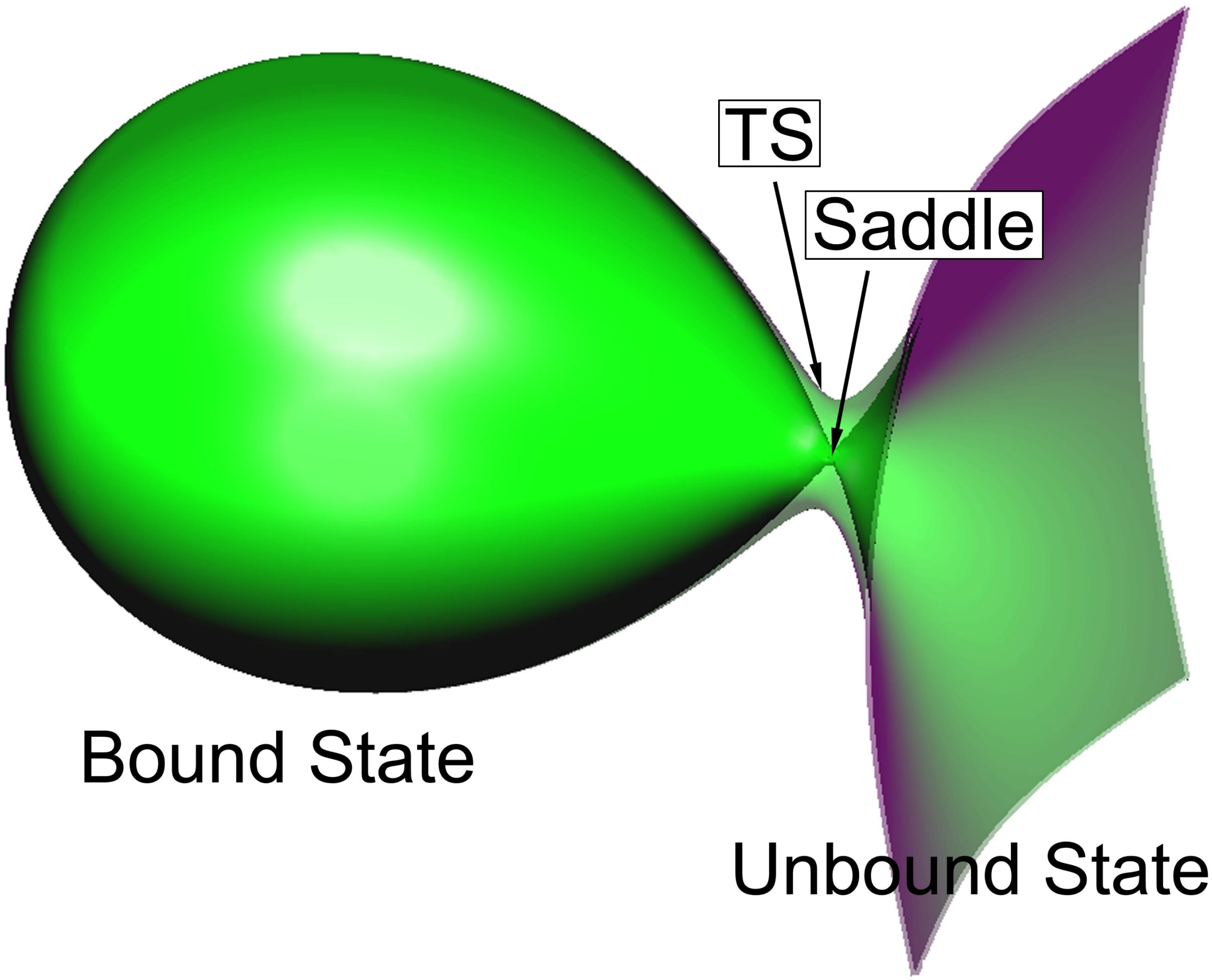
Transition State Theory





- Transition State: Joins Reactants & Products
  - **Bottleneck near rank-1 saddle**
  - **Opens for energies larger than saddle**
- TST Assumes Unstructured Phase Space
  - **Even Chaotic Phase Space is Structured**

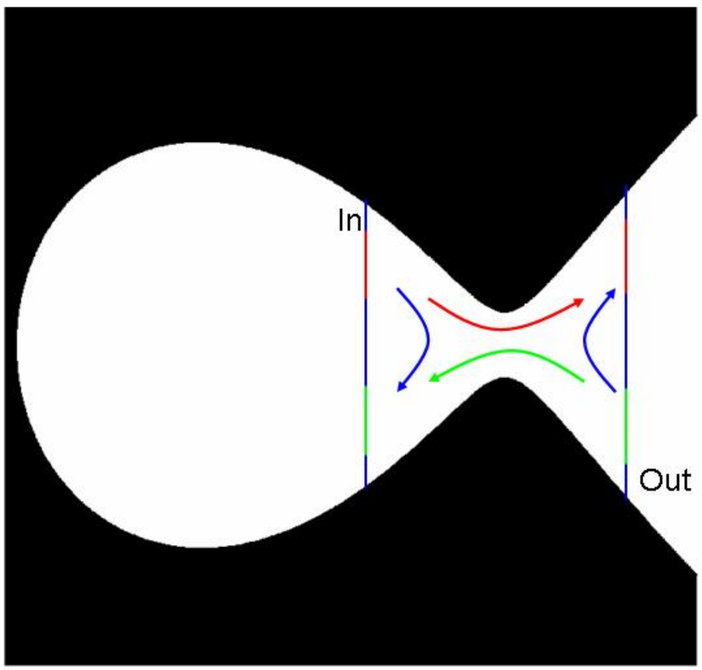
What is a Scattering Reaction?

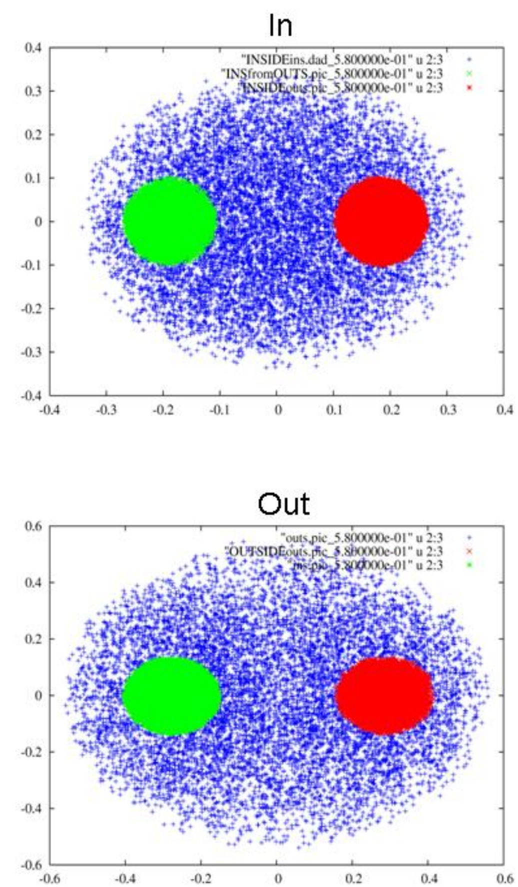


- Bound vs. Unbound States (Hill Region)
- Zero Angular Momentum not always valid

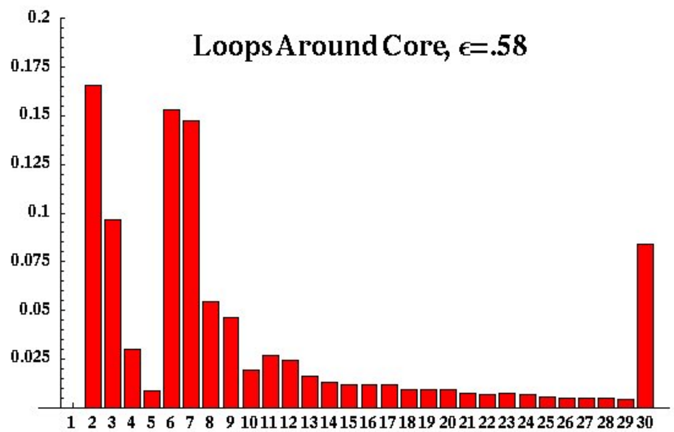
Example - Rydberg Atom

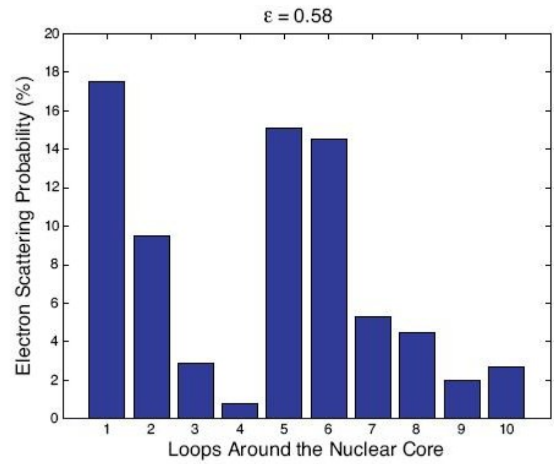
$$H = \frac{1}{2}\left(p_x^2 + p_y^2 + p_z^2\right) + \frac{1}{2}\left(xp_y - yp_x\right) + \frac{1}{8}\left(x^2 + y^2\right)$$
$$-\epsilon x - \frac{1}{\sqrt{x^2 + y^2 + z^2}}$$

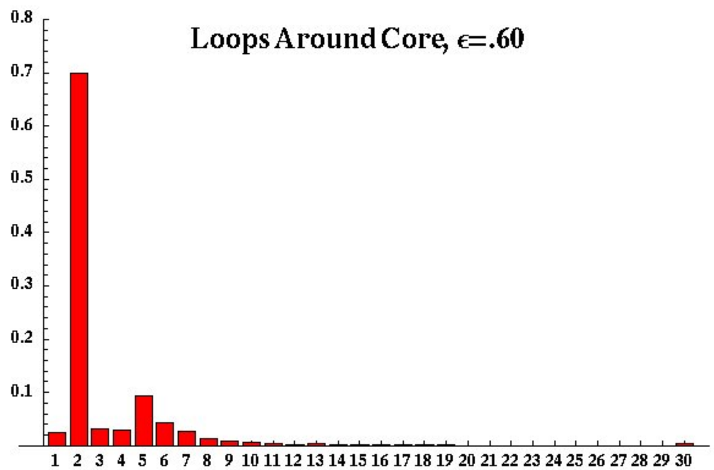


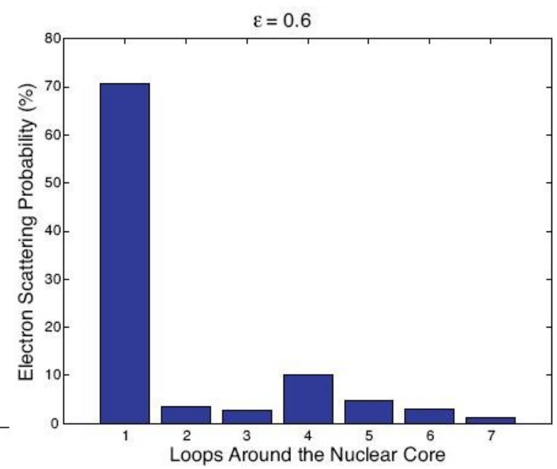


Rydberg Atom Cont'd







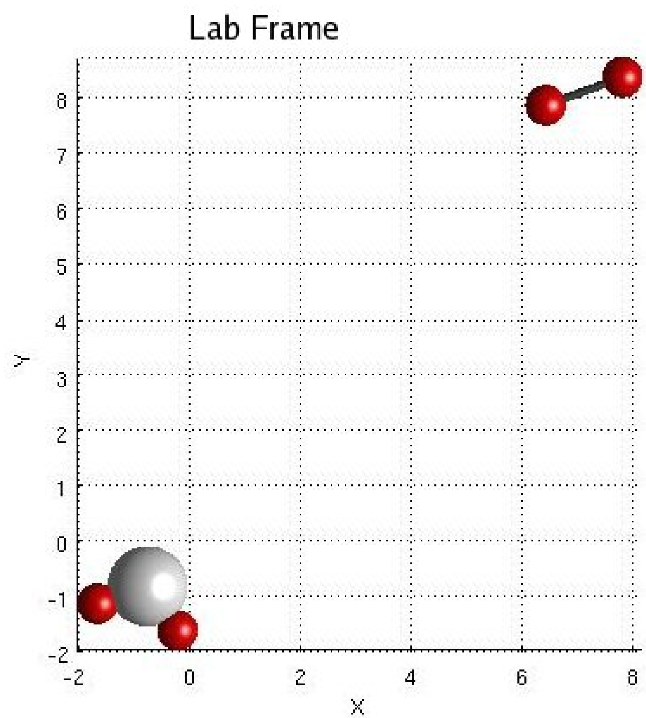


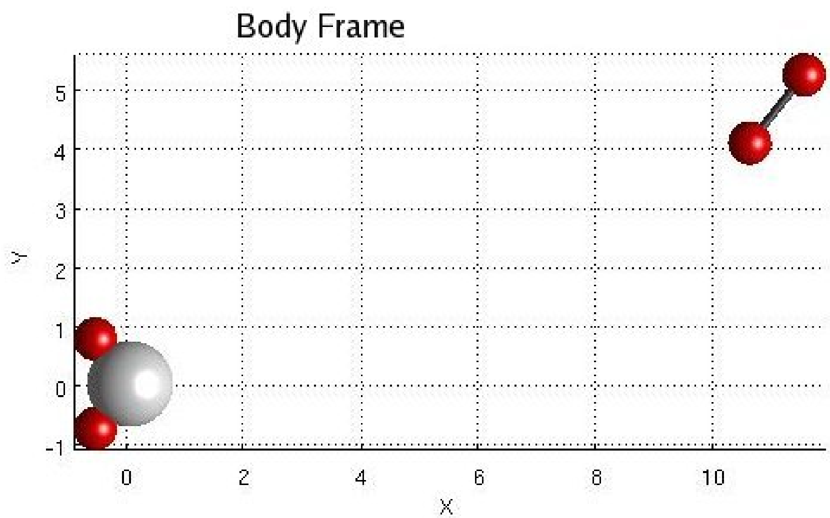
- **~3 minutes :: 4,000 pts :: $< .5\%$ error**
- **~1 hour :: 140,000 pts :: $< .1\%$ error**
- **~2 days :: 1,000,000 pts ::**

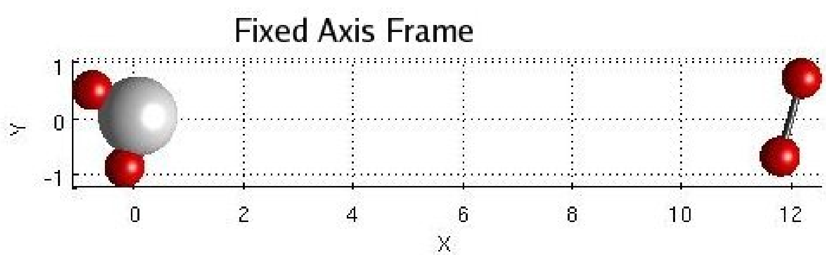
Planar Scattering of H_2O-H_2

$$H = \frac{p_R^2}{2m} + \frac{(p_\theta - p_\alpha)^2}{2mR^2} + \frac{(p_\alpha - p_\beta)^2}{2I_a} + \frac{p_\beta^2}{2I_b} + V$$

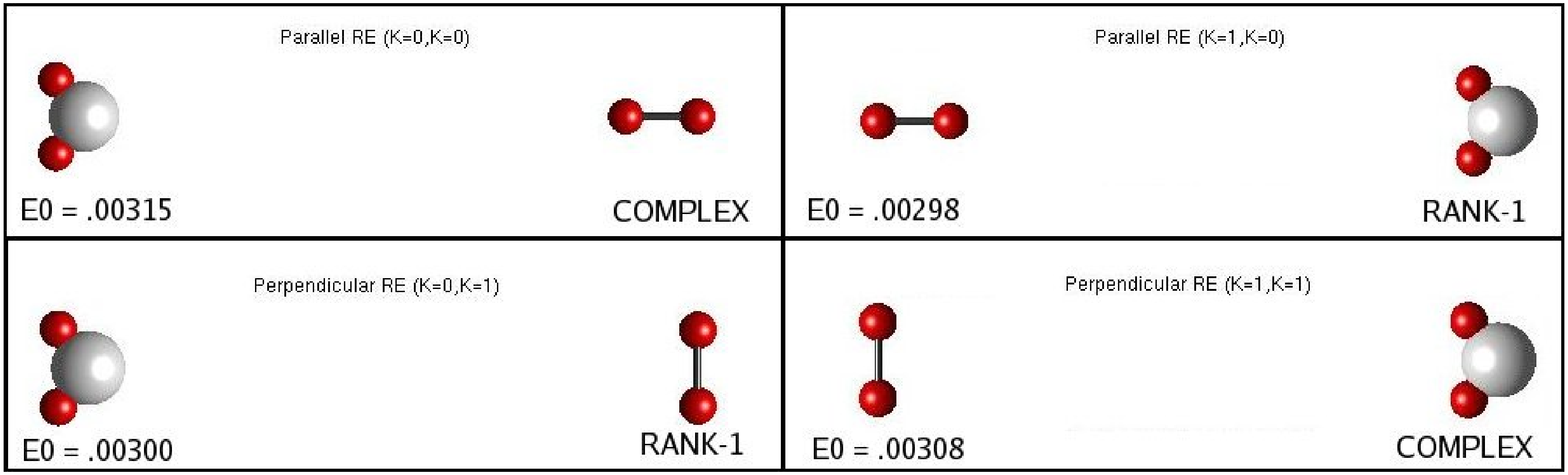
- V = **dipole/quadrupole + dispersion + induction + Leonard-Jones. (Wiesenfeld, 2003)**
- **Reduce out θ and work on $p_\theta \equiv J > 0$ level set.**

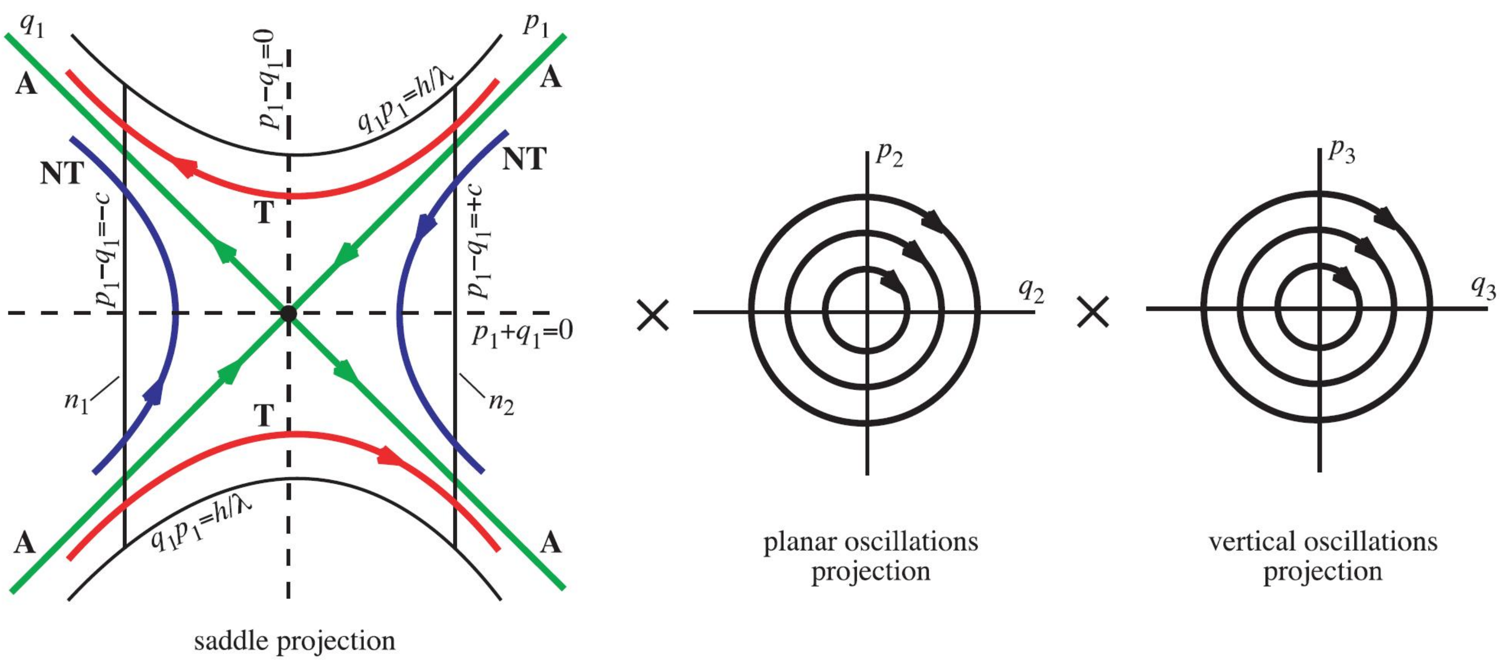






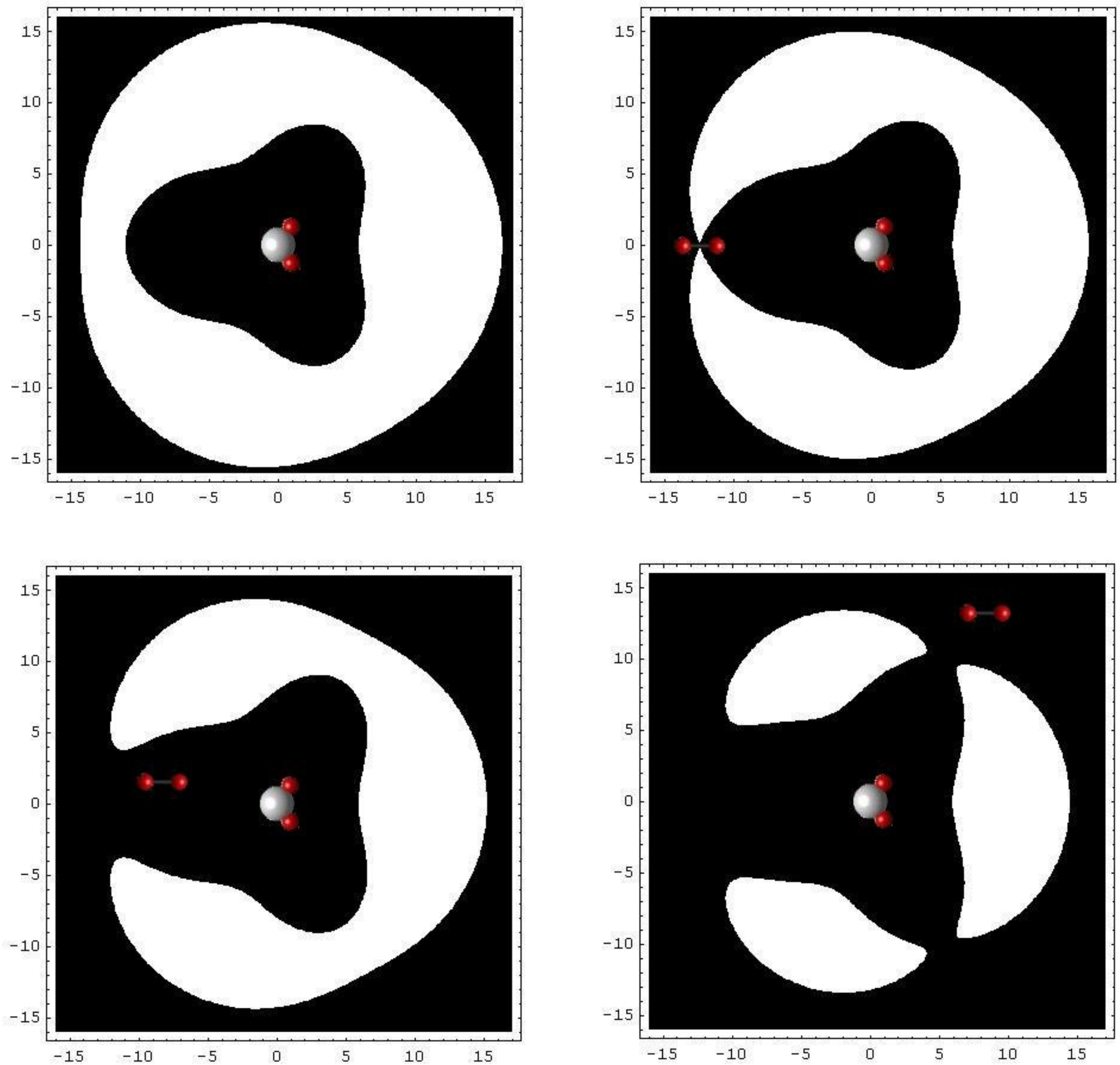
H_2O-H_2 Saddles



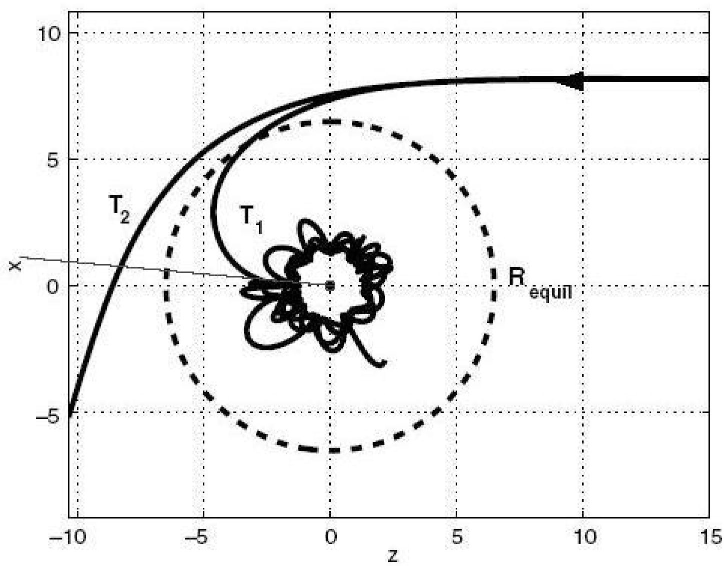


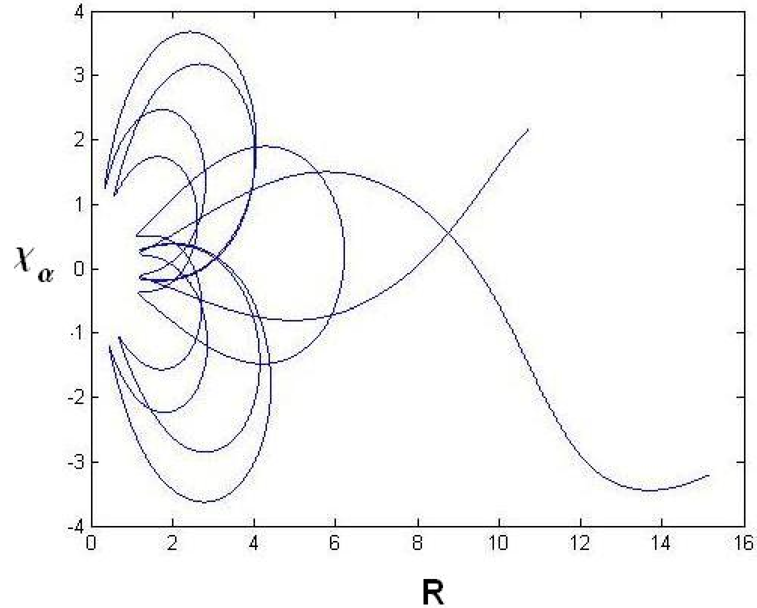
Linearization near rank-1 saddle

H_2O-H_2 Hill Region



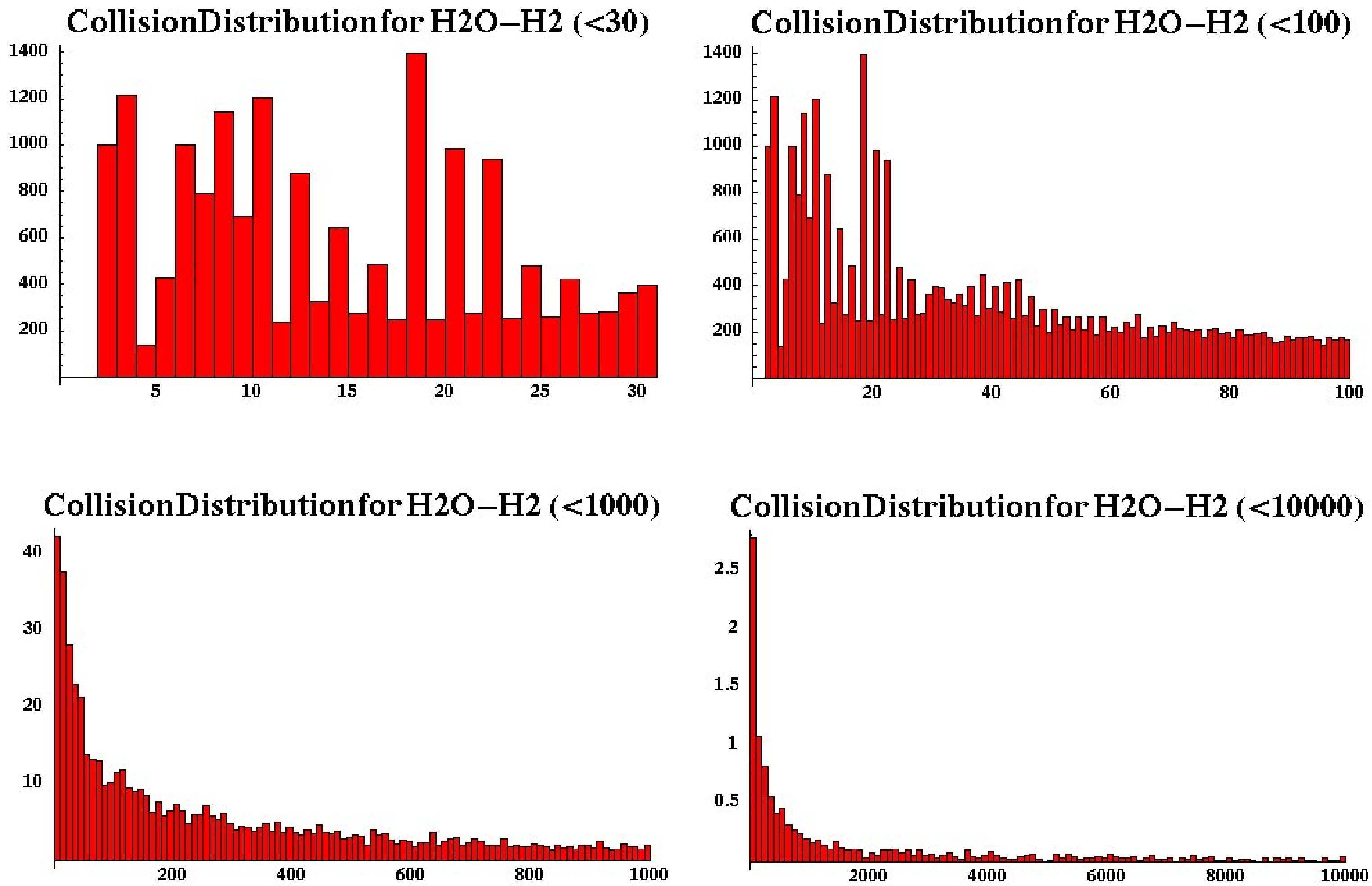
H_2O-H_2 Collision Dynamics





- ☐ Unrealistic Potential?
- ☐ Numerically Volatile Collisions
- ☐ Is Non-Scattering Reaction Occurring?
- ☐ More Realistic Potential Surface (Wiesenfeld)

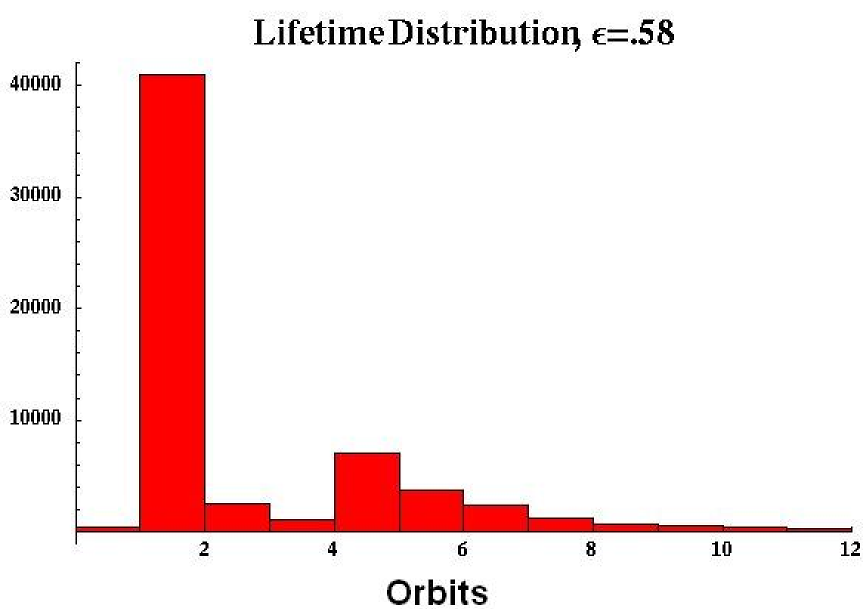
H_2O-H_2 Lifetime Distribution

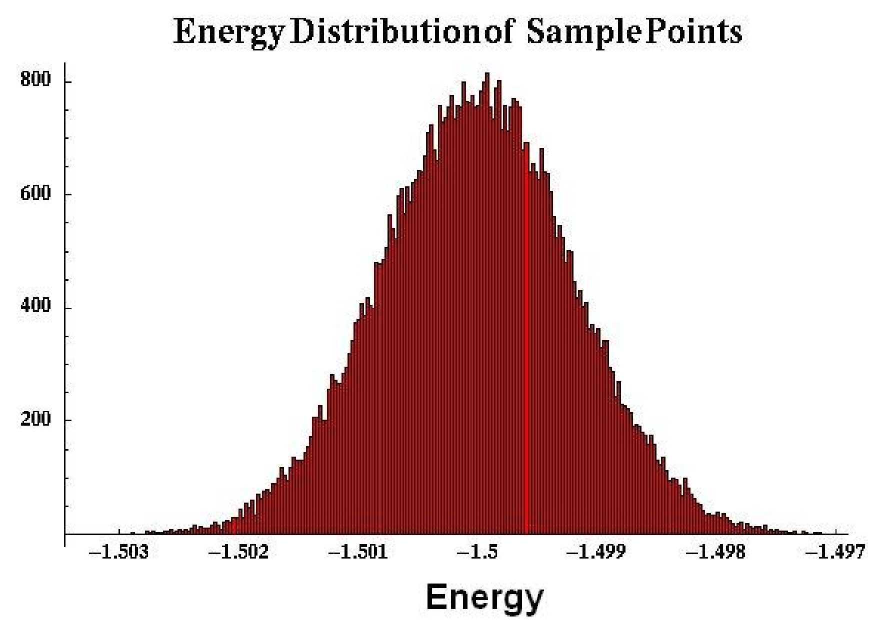


- **Locally structured (fine scale)**
- **Globally RRKM (coarse scale)**
  - Does structure persist w/ error in energy samples?

Gaussian Energy Sampling

- Experimental verification of lifetime distribution
  - **Fixed energy slice is not realistic**
  - **Gaussian around target energy is more physical**
  - **Do nonRRKM features persist?**

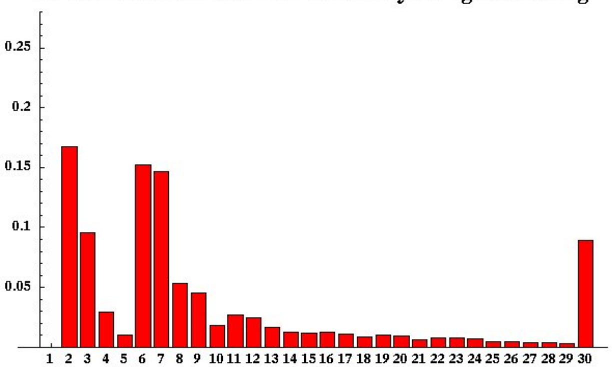




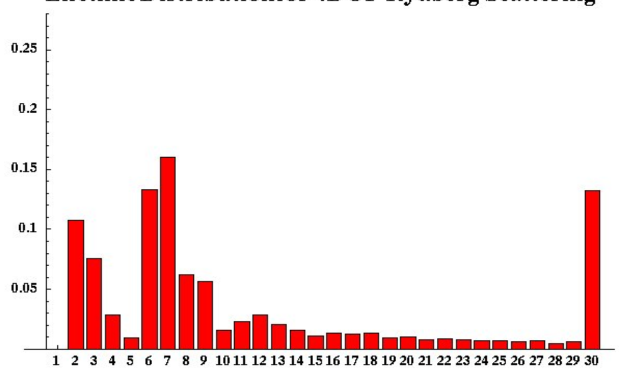
$\geq$ 3 DOF Rydberg Analog

$$H = \frac{1}{2}\left(p_x^2 + p_y^2 + p_z^2 + p_w^2\right) + \frac{1}{2}\left(xp_y - yp_x\right) + \frac{1}{8}\left(x^2 + y^2\right) - \epsilon x - \frac{1}{\sqrt{x^2 + y^2 + z^2 + w^2}}$$

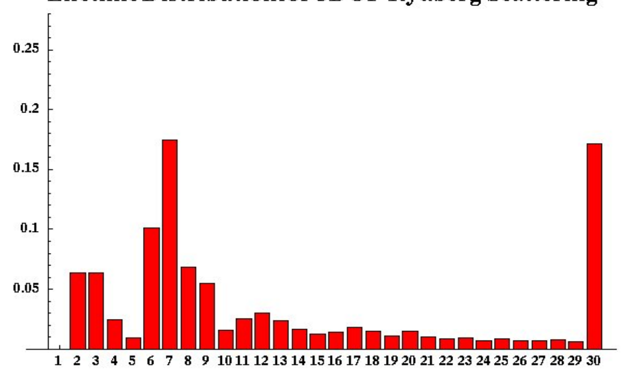
Lifetime Distribution for 3DOF Rydberg Scattering



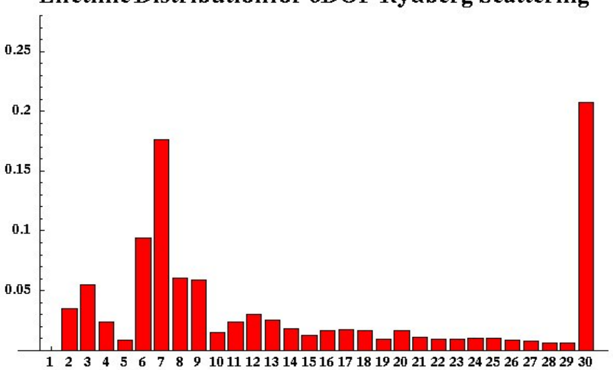
Lifetime Distribution for 4DOF Rydberg Scattering



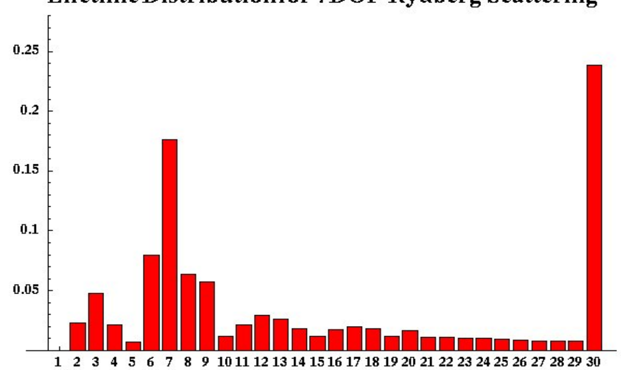
Lifetime Distribution for 5DOF Rydberg Scattering



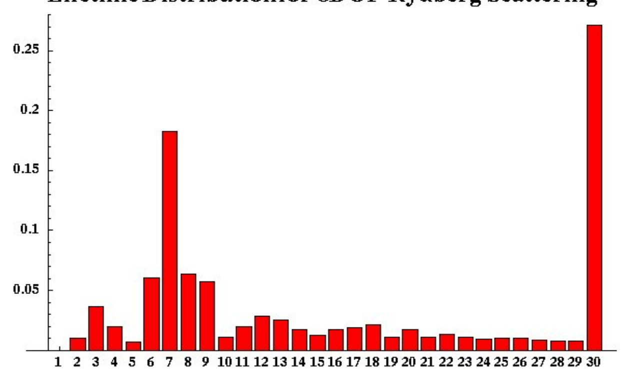
Lifetime Distribution for 6DOF Rydberg Scattering



Lifetime Distribution for 7DOF Rydberg Scattering



Lifetime Distribution for 8DOF Rydberg Scattering

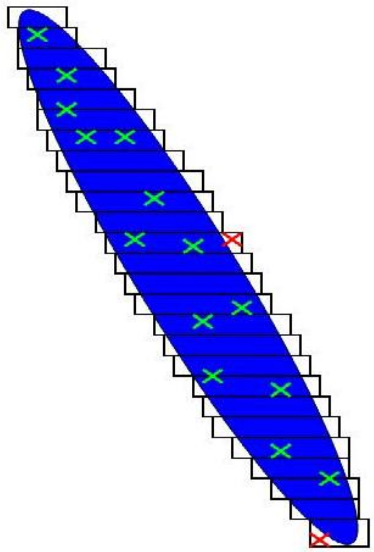


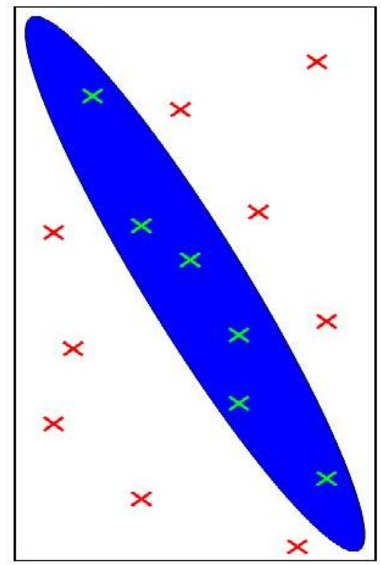
Comparison of Methods

- High Order Normal Form Expansion
  - **Compute Transit Tubes directly**
  - **NF expansion becomes involved for > 3 DOF**
- Almost Invariant Set Methods (GAIO)
  - **Transfer operators on box subdivisions**
  - **Increasing memory demands w/ higher DOF**
- Bounding Box Method
  - **Lifetime Distribution essentially 1D problem**
  - **Scales well to higher DOF systems**
  - **Integration & sampling become bottleneck**

Future Work

- Tighter Bounding Box





- Variational Integrator
  - **Larger time steps, faster runtime**
  - **Computes collisions more accurately**
  - **Bulk of computation is integration**
- Asteroid Capture Rates

Conclusions & Open Questions

- Conclusions
  - **Bounding Box Method is very efficient**
  - **Requires minor modification for new systems**
  - **Remains fast for high DOF systems**
- Next Steps
  - **Apply method to higher DOF chemical system**
  - **Obtain experimental verification of method**
- Open Problems
  - **Is there an estimate for how small energy must be for linear dynamics to persist?**
  - **Perron-Frobenius operator (coarse grained reaction coordinate)**
  - **Apply tube dynamics to stochastic models**
  - **Solve Rank-2 sampling problem (non-compact)**

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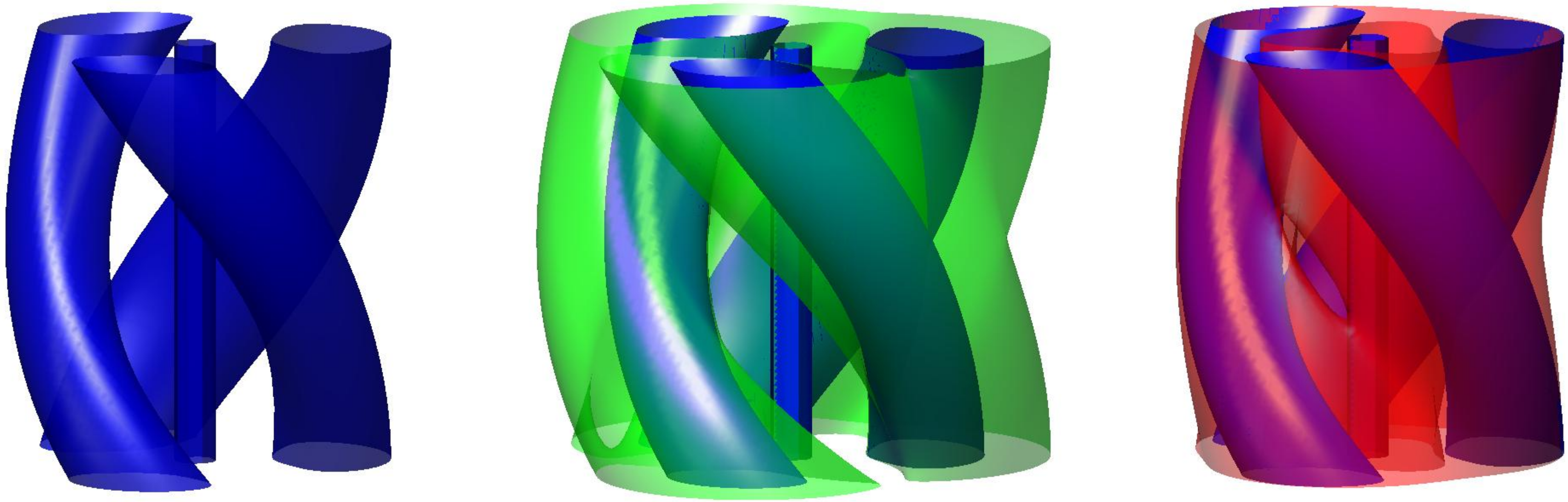
The End



Questions...

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