Transport in Hamiltonian Systems With Two or More Degrees of Freedom

Shane Ross

Wang Koon and Jerry Marsden (CDS), Martin Lo (JPL)

April 18, 2001
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 → 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

"Bound"

Nucleus

"Free"
Partition the Phase Space

- Comet near the Sun and Jupiter

Potential

Configuration Space

$U_{\text{eff}}$

$L_1, L_2, L_3, L_4, L_5$

Sun

Jupiter
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
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 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 $t > 0$. 

\begin{figure}[h]
\centering
\includegraphics[scale=0.5]{diagram.png}
\caption{Regions $R_1, R_2, R_3, R_4$}
\end{figure}
Some quantities we would like to compute are:

- $T_{i,j}(t) = \text{the total amount of species } S_i \text{ contained in region } R_j \text{ at time } t$
- $F_{i,j}(t) = \frac{dT_{i,j}(t)}{dt} = \text{the flux of species } S_i \text{ into region } R_j \text{ at time } t$
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

$$\oint_{\mathcal{L}} p \cdot dq = \int_{\mathcal{A}} dp \wedge dq = \text{constant}$$
\[ \sum_{i=1}^{N} \sigma_i \int_{A_i} dp_i dq^i = \text{constant on an energy surface} \]
Suppose there is another \((2N - 1)\)-dimensional surface \(Q\) that is transverse (i.e., nowhere parallel) to the flow in some local region.

The Poincaré section \(S\) is the \((2N - 2)\)-dimensional intersection of \(M_E\) with \(Q\).
Example for $N = 2$

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

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

- Rotating Frame
- Comet
- Sun
- Jupiter
- Position Space
- Effective Potential

$U^{\text{eff}}$
Look at fixed energy

Case 1: \( E < E_1 \)

Case 2: \( E_1 < E < E_2 \)

Case 3: \( E_2 < E < E_3 \)

Case 4: \( E_3 < E < E_4 = E_5 \)

Position Space Projections
3-Body Problem (2D)

Partition the energy surface

Position Space Projection
Look at motion near “saddle points”
Potential Barriers

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

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

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.
□ For fixed energy $H = \hbar$, 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.,

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

Note that $\mathcal{M}_\hbar \simeq S^1$, a periodic orbit.
Local Dynamics

Four cylinders of asymptotic orbits: the stable and unstable manifolds $W^s_\pm(M_h), W^u_\pm(M_h)$.

Stable Manifold (orbits move toward the periodic orbit)

Unstable Manifold (orbits move away from the periodic orbit)
Cylinders separate transit from nontransit orbits.

Define mappings between “bounding spheres” on either side of the potential barrier.
Stable and unstable manifold tubes

- Control transport through the potential barrier.
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.
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.
**Transition Probabilities**

- **Example:** Comet transport between outside and inside of Jupiter
Look at Poincaré section intersected by both tubes. Choosing surface \( \{ x = \text{constant}; p_x < 0 \} \), we look at the canonical plane \((y, p_y)\).
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 \((y, p_y)\)
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 transforms 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:
  \[
  I_j = q_j^2 + p_j^2, \quad j = 1, \ldots, N - 1, \quad \text{and} \quad I_N = q_N p_N.
  \]

The \( N \) Canonical Planes
\[ N = 3 \text{ or More} \]

- 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 \( \mathcal{M}_h \cong S^{2N-3} \), 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)
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


