Chaotic transition states in tri-atomic molecules

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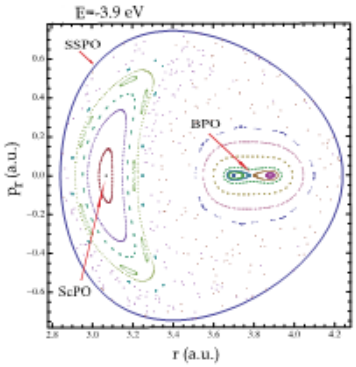

It is an important problem in chemistry to predict what the outcome of a reaction will be: Will a reaction occur, what product will be formed, and under what conditions? To make that decision, you need to know the boundaries between configurations that lead to a reaction and those that don't. These boundaries are smooth surfaces that are known as invariant manifolds. Once they are known, you have all important information about the dynamics of a reaction.

Tri-atomic molecules are the ideal examples to investigate these structures. While they are "simple" examples in chemical terms, they are important model systems for more complex chemical reactions and their dynamics is rich enough that in many cases we don't understand it in detail. This is true, in particular, where the dynamics becomes chaotic and we have to deal with fractal structures. An important obstacle is that our numerical methods for calculating the invariant manifolds aren't quite powerful enough.

In this project you will study the dynamics of atoms in terms of classical mechanics. You will numerically compute the solutions of Newton's (or Hamilton's) equations of motion and see how individual trajectories fit together to form larger structures. You will develop the numerical methods to compute invariant manifolds and use them to elucidate how, and why, exactly chaotic dynamics arises in chemical reactions. You will learn how to obtain data relating to actual chemical reactions through quantum chemistry calculations.

References:

1. M. Feldmeier *et al:* Invariant Manifolds and Rate Constants in Driven Chemical Reactions. J. Phys. Chem. B **123** (2019) 2070.
2. F. Revuelta Peña *et al:* Transition state theory for activated systems with driven anharmonic barriers. J. Chem. Phys **147** (2017) 074104.
3. A. Allahem and T. Bartsch: Chaotic dynamics in multidimensional transition states. J. Chem. Phys. **137** (2012) 214310.