Interacting transition states for reactions with several pathways

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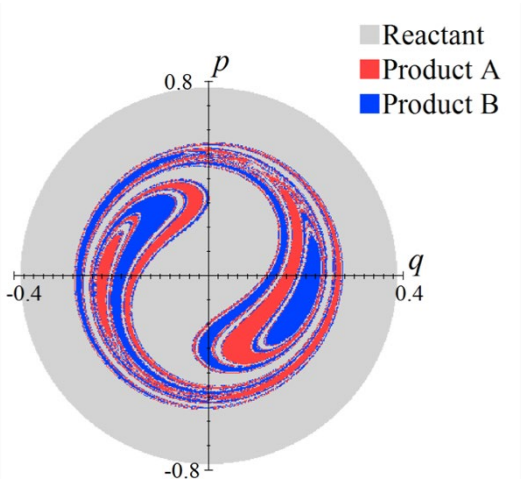

When studying chemical reactions, we do not only want to predict whether a reaction will happen at all (will a given product be formed?) but we often want to gain a detailed understanding of the underlying reaction mechanism (How do we get to the product?) In many cases, there is only one possible reaction path, and then we understand the dynamics of the reaction quite well. Sometimes, however, for low reaction energies there are two competing pathways from the reactants to products that merge into a single pathway as the energy goes up. While we understand the low-energy regime fairly well, we don't know how the merging of pathways happens and what kind of dynamics occurs in the high-energy regime beyond it.

In this project you will study the dynamics of atoms in terms of classical mechanics. You will investigate how the transition from two pathways to one happens. To identify a reaction channel, 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. You will numerically compute these manifolds for simple reactions and/or model systems and see how they change when the two pathways merge. You will learn how to perform quantum chemistry computations to bridge between this formal description and actual chemical reactions.

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. Junginger *et al:* Symmetry-breaking thermally induced collapse of dipolar Bose-Einstein condensates. Phys. Rev. A **86** (2012) 023632.