Handling large expressions symbolically in transition state theory

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Abstract

In this talk we show the normal form approach as a way of getting an analytical handle on geometric objects, such as normally hyperbolic invariant manifolds (NHIM), and the breakthrough this is in chemistry, as well as in celestial mechanics problems. Computer visualization is used in order to "see" these objects. We illustrate the technique through several examples borrowed from chemistry and astrodynamics. Concretely, we show how to determine analytically the transition state (TS) in chemical reactions. For that we calculate the normal form and transform the original three-degree-of-freedom (3DOF) Hamiltonian to a 0DOF one. These expressions need to be known very accurately, so one carries out the computations to a high degree, therefore using very large formulae. In fact, we are able to construct three asymptotic integrals of the original Hamiltonian by inverting the normal form transformation. Moreover, we calculate in the original system the three-dimensional NHIM, its stable and unstable manifolds, as well as the transition state. We compute trajectories that start on the NHIM in the five-dimensional energy surface. Besides, we determine trajectories in either the forward or backward stable and unstable manifolds associated to the NHIM. These trajectories are simply chosen and computed from the normal form vector field. The normal form transformation then allows us to visualize them in the original coordinates. Thus, we have complete control and knowledge of the exact dynamical trajectories near the TS in a 3DOF system. For the calculations we make use of the commercial software MATHEMATICA.