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Transition State Theory for Higher-Rank Saddles

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Recent developments in transition state theory have lead to a geometric characterization of molecular reactions in phase space. Central to this new characterization is the existence of codimension-one surfaces in the energy shell; these invariant surfaces guide reacting trajectories through sections of no return, the transition states. The existence of codimension-one invariant surfaces has only been shown in the vicinity of rank-one saddles, i.e., near fixed points with one stable and one unstable direction in addition to neutrally stable directions. For higher-rank saddles, the current framework of geometric transition state theory has remained inapplicable. Here we describe a generalization of the theory to saddles of arbitrary rank. As an application, we describe the nonsequential ionization of helium atoms, a problem with a rank-two saddle.