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Dynamical Reaction Theory and Time Series Analysis

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We provide an overview of the recent progress of the dynamical theory of reactions. After summarizing the conventional statistical reaction theory, we explain the basic concepts underlying the dynamical theory, i.e., normally hyperbolic invariant manifolds (NHIMs) and the Arnold web. Then, we go on to discuss the dynamical theory using these concepts. Here, we discuss the following three processes: (i) redistribution of energy among vibrational modes in the well, (ii) going over the potential saddle, and (iii) dynamical connection among multiple saddles.

In particular, we focus our attention to those processes where limitations of the conventional statistical theory become manifest. We will also discuss time series analysis to extract dynamical information from molecular dynamics simulations involving multi-dimensional Hamiltonian systems.

Keywords: Phase Space Structures, Reaction Theory, Time Series Analysis.