Phase Space Transition States for Deterministic Thermostats
GREGORY EZRA, Cornell University, STEPHEN WIGGINS, Bristol University
— We describe the relation between the phase space structure of Hamiltonian and non-Hamiltonian deterministic thermostats. We show that phase space structures governing reaction dynamics in Hamiltonian systems, such as the transition state, map to the same type of phase space structures for the non-Hamiltonian isokinetic equations of motion for the thermostatted Hamiltonian. Our results establish a general theoretical framework for analyzing thermostat dynamics using concepts and methods developed in reaction rate theory. Numerical results are presented for the isokinetic thermostat.