Summary

Algorithmic approaches for the identification of essential statistical behavior have successfully been applied to study deterministic dynamical systems and molecular systems in a Hamiltonian context.

This thesis unifies and extends theory and algorithmic concepts from the formerly considered special classes of dynamical systems to the broader class of Markovian systems. We provide a detailed analysis of metastability and a new theoretical justification of the transfer operator based approach to metastability (Sec. 3). It is based on an instructive theorem (Theorem 3.1) specifying the relation between eigenvalues close to 1 and the existence of a decomposition into metastable subsets. This thesis contributes new links between spectral properties of transfer operators and well established Doeblin and ergodicity conditions for Markov processes and operators (Thms. 4.13, 4.24, 4.31).

We obtain a rather complete understanding in the $L^1(\mu)$ setting for general Markov processes (Secs. 4.2, 4.3), and for the $L^2(\mu)$ setting in the case of reversible Markov processes (Sec. 4.4). This allows us to successfully extend the concepts to new model systems, and we investigated for the first time the essential statistical behavior of the Langevin and the Smoluchowski equation in comparison with the Hamiltonian system with randomized momenta. We furthermore suggested an algorithmic indicator for the essential spectral radius (Sec. 5.1), which proved to be useful in application to our test system.

We outlined the strategies for studying larger molecular systems and successfully demonstrate its application to the study of the triribonucleotide r(ACC) (Sec. 7).