Metastability, Spectra, and Eigencurrents of Lennard-Jones Clusters

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The concept of metastability and its relation to the structure of the spectrum has caused a lot of interest in recent years. I will introduce computational tools for spectral analysis of large stochastic networks representing energy landscapes of atomic and molecular clusters. In such networks, the pairwise transition rates vary exponentially and render the calculation of small eigenvalues and corresponding eigenvectors challenging. The proposed approach consists of two steps: (i) computation of the zero-temperature asymptotics of eigenvalues and eigenvectors, and (ii) a continuation technique for finite temperatures. This methodology will be applied to the investigation of networks representing Lennard-Jones clusters created by Wales's group. I will give detailed descriptions of escape processes from the major metastable sets at different of temperatures in terms of eigencurrents and demonstrate a superexponential growth of the escape rates.