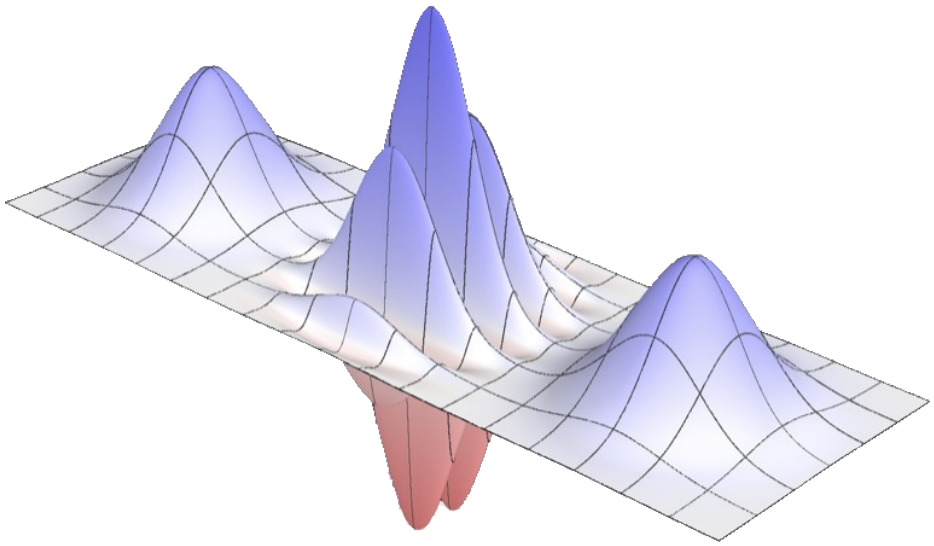
E-CAM State-of-the-Art Workshop

Recent developments in Quantum Dynamics



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Semiclassical molecular dynamics for spectroscopic calculations of high dimensional and condensed phase molecular systems

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I will present some novel semiclassical methods designed for spectroscopic IR calculations of high dimensional and/or condensed phase systems. These methods are based on a “divide-and-conquer” approach [1-3], where the full dimensional spectra are obtained as a composition of several lower dimensional ones or exploit hierarchically the different levels of accuracy of different semiclassical propagators [4-6]. All methods are within 10-20 wavenumbers Mean Absolute Error average respect to the exact or experiments when available[7,8], and are amenable to ab initio molecular dynamics simulations [9-11].

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