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

Abstract:

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]

References

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