Quantum Vibrational Spectroscopy of Biomolecular Systems through Divide-and-Conquer Semiclassical Dynamics

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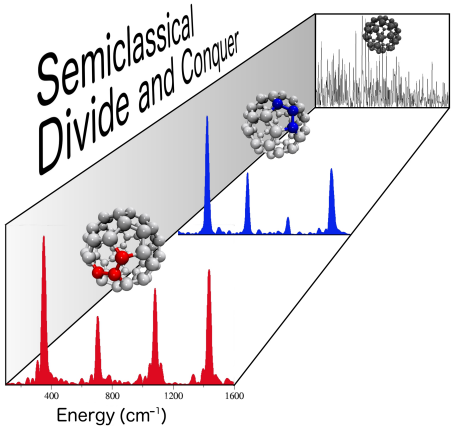

Semiclassical dynamics has long been known to be able to calculate accurately vibrational power spectra of small, isolated molecules with inclusion of quantum effects like zero-point energies, overtones, and quantum resonances.[1,2] Recent methodological advances have permitted application of semiclassical spectroscopy to larger molecular systems up to several dozens of atoms,[3] simulation of IR spectra,[4] and determination of vibrational eigenfunctions.[5]

In this talk I will briefly introduce the divide-and-conquer semiclassical initial value (DC SCIVR) method and illustrate a few relevant applications of biomolecular interest. Specifically, a study of water clusters, aimed at determining the minimum number of water molecules needed to solvate a central one, will point out the possibility to deal with the solvation issue.[6] An investigation of glycine will allow me to describe the vibrational features of this small but quaint amino acid, whose role is widely debated in the biochemical and astrochemical communities.[7,8,9] Simulation of some relevant spectral features of nucleosides will be used to compare results based on precise ab initio on-the-fly semiclassical dynamics with those relying on force fields, providing for the latter a quantum based assessment of their accuracy.[10] To conclude an on-going study of solvated thymidine will be briefly introduced.

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