VISTA Seminar

Seminar 26

October 28, 2021

10:00 am – 11:30 am EDT / 2:00 – 3:30 pm GMT / 4:00 pm – 5:30 pm Paris

TOC:

Semiclassical Initial Value Representation Molecular Dynamics for Spectroscopy

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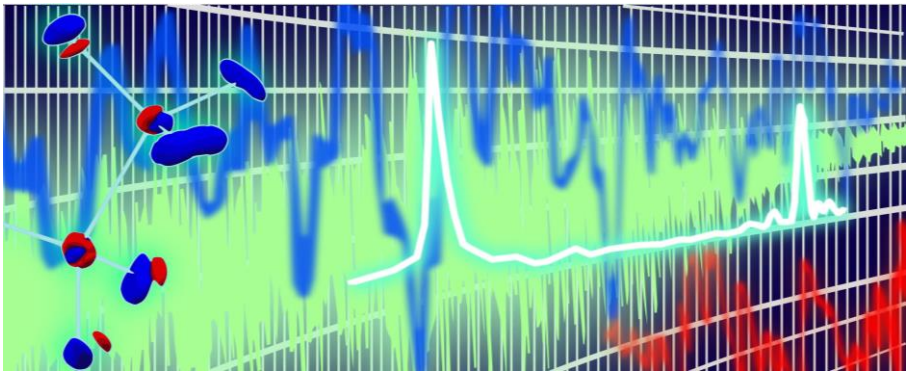

Semiclassical Initial Value Representaiton (SCIVR) molecular dynamics has been known since a long time to be able to calculate accurately vibrational power spectra of small, isolated molecules with inclusion of quantum effects, such as zero-point energies, overtones, tunneling splittings, and quantum resonances.[1] Our group introduced some methodological advances that have permitted the application of semiclassical spectroscopy to larger molecular systems up to several dozens of atoms, simulation of IR spectra, and determination of vibrational eigenfunctions.
In this talk I will briefly recall the SCIVR approximation and introduce the divide-and-conquer semiclassical initial value (DC SCIVR)[2] method with some applications. Specifically, I will show how we implemented DC SCIVR with a machine learning algorithm and applied it to NMA spectra calculations, how SCIVR can deal with the solvation issue by studying water clusters[3]. We also deal with molecular adsorption on TiO2(101) Anatase surface using direct ab initio molecular dynamics by reproducing spectra of adsorbed molecules. Then, simulations of some relevant spectral features of nucleobases, nucleosides and an on-going study of solvated thymidine will be used to compare results based on precise ab initio on-the-fly semiclassical dynamics with those relying on force fields.[4,5]

References:
[1] W.H. Miller, *Proc. Natl. Acad. Sci. U.S.A.* **102**, 6660 (2005).
[2] M. Ceotto, G. Di Liberto, and R. Conte, *Phys. Rev. Lett.* **119**, 010401 (2017).
[3] A. Rognoni, R. Conte, and M. Ceotto, *Chemical Sciences* **12**, 2060 (2021).
[4] F. Gabas, G. Di Liberto, R. Conte, and M. Ceotto, *Chemical Science* **9** (41), 7885-8026 (2018).
[5] C. Aieta, M. Micciarelli, G. Bertaina, and M. Ceotto, *Nature Communications* **11**, 1-9 (2020).

A novel method to prevent zero-point energy leak in classical trajectory simulation

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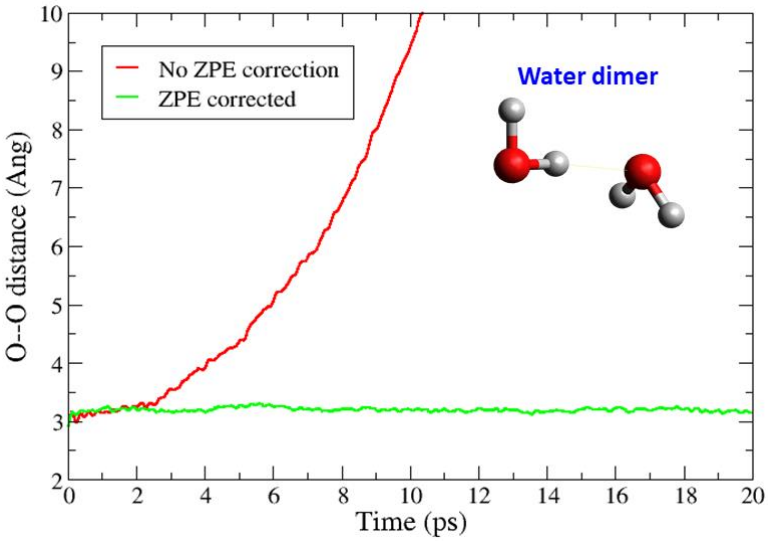

The problem associated with the zero-point energy (ZPE) "leak" in quasiclassical trajectory calculations are well known. This phenomenon can lead to unphysical results, such as forming products without the ZPE in the internal vibrational degrees of freedom (DOFs). The ZPE leakage also permits reactions below the quantum threshold for the reaction. In contrast, a quantum mechanical wavepacket moves over the saddle point towards products with vibrational mode energies greater or equal to their ZPE values. In this talk, a new method inspired by the Lowe-Andersen thermostat will be shown to prevent energy dipping below a threshold in the internal vibrational DOFs. The idea is to pump the leaked energy to the corresponding internal DOF, taken from the other internal DOFs. The other vibrational modes act as a pool from which energy can be taken to compensate for the leakage of vibrational energy in the relevant internal DOF, hence preventing the latter from falling below a threshold value, namely, ZPE. Thus, the energy is redistributed over the DOFs conserving the total energy of the system.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 26
Time: Oct 28, 2021 10:00 AM Eastern Time (US and Canada)

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