VISTA Seminar

Seminar 55

September 13, 2023

10:00 am – 11:30 am EST / 3:00 – 4:30 pm GMT London / 4:00 pm – 5:30 pm CET Paris / 10 pm CST Beijing

TOC:

Classical Molecular Dynamics Simulations of Electronically Non-Adiabatic Processes

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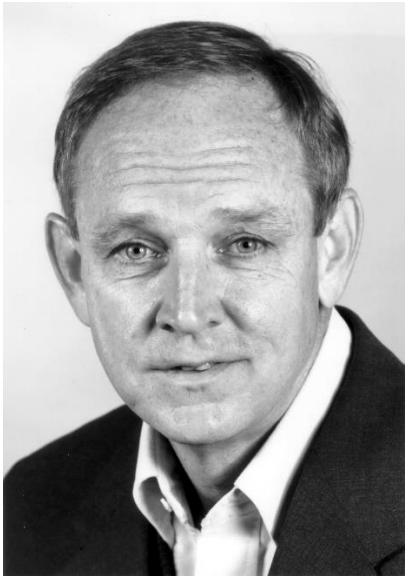

A recently described symmetrical quasi-classical (SQC) windowing methodology for classical trajectory simulations has been applied to the Meyer-Miller (MM) model for the electronic degrees of freedom in electronically non-adiabatic dynamics. The approach treats nuclear and electronic degrees of freedom (DOF) equivalently (i.e., by classical mechanics, thereby retaining the simplicity of standard molecular dynamics), providing ``quantization'' of the electronic states through the symmetrical quasi-classical (SQC) windowing model. The approach is seen to be capable of treating extreme regimes of strong and weak coupling between the electronic states, as well as accurately describing coherence effects in the electronic DOF (including the de-coherence of such effects caused by coupling to the nuclear DOF). It is able to provide the full electronic density matrix from the one ensemble of trajectories, and the SQC windowing methodology correctly describes detailed balance (unlike the traditional Ehrenfest approach). Calculations can be (equivalently) carried out in the adiabatic or a diabatic representation of the electronic states, and most recently it has been shown that a modification of the canonical equations of motion in the adiabatic representation eliminates (without approximation) the need for second-derivative coupling terms.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 55
Time: Sep 13, 2023 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/96159187451?pwd=L0VBQXY2ZDI4bG1NYUhnYUs1RW1zZz09

Meeting ID: 961 5918 7451
Passcode: 453952