VISTA Seminar

Seminar 29

December 9, 2021

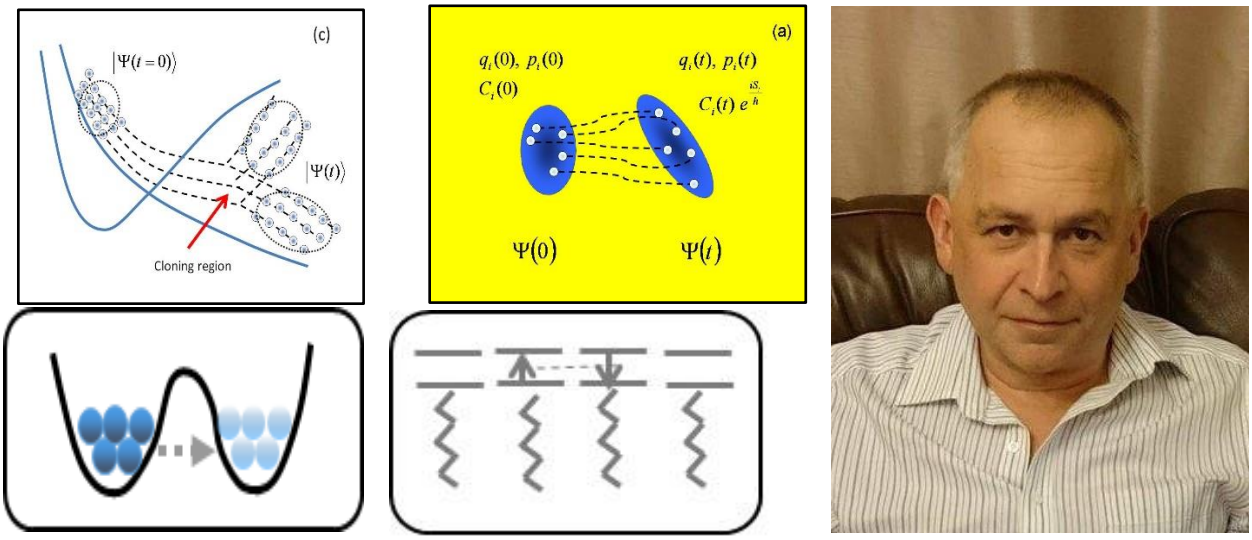
10:00 am – 11:30 am EST / 3:00 – 4:30 pm GMT / 4:00 pm – 5:30 pm Paris

TOC:

A brief overview of trajectory guided Coherent State basis sets methods of quantum dynamics with examples of applications in Photochemistry and in Physics.

Dmitrii V Shalashilin

School of Chemistry, University of Leeds. LS2 9JT Leeds, UK
Email: d.shalashilin@leeds.ac.uk



An overview of existing methods which use trajectory guided grids of Coherent States will be given and the technical details of Multiconfigurational Ehrenfest approach will be discussed. Single trajectory semiclassical Ehrenfest methods often are not very accurate, but Ehrenfest trajectories work very well to guide quantum basis sets. In chemistry the trajectory guided random grids of Gaussian Coherent States are routinely used to simulate quantum dynamics in ultrafast photochemistry in a manner similar to classical molecular dynamics, but with the difference that an ensemble of trajectories is used instead of a single trajectory[1]. With the right sampling techniques they can yield well converged results for molecules with tens of vibrations, treating all nuclear degrees of freedom on a fully quantum level[2]. Similar methods based on Gaussian Coherent States can be used in physics to simulate the dynamics of ensembles of Bose particles described by second quantisation Hamiltonians[3]. Other types of Coherent States, such as Coherent States of two level systems can be used to describe fermions[4] and to obtain Born-Oppenheimer electronic energies and coupled qubits.

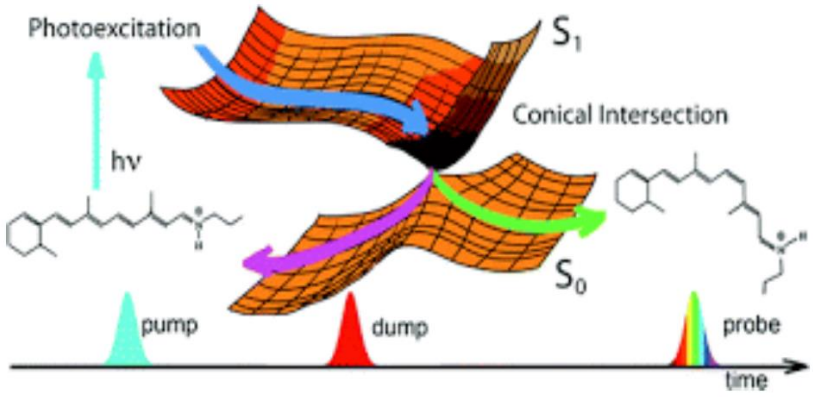
References

1. Makhov, D. V.; Symonds, C.; Fernandez-Alberti, S.; Shalashilin, D. V., Ab initio quantum direct dynamics simulations of ultrafast photochemistry with Multiconfigurational Ehrenfest approach. *Chemical Physics* **2017,** *493*, 200-218.
2. Symonds, C.; Kattirtzi, J. A.; Shalashilin, D. V., The effect of sampling techniques used in the multiconfigurational Ehrenfest method. **2018,** *148* (18), 184113.
3. Green, J. A.; Shalashilin, D. V., Simulation of the quantum dynamics of indistinguishable bosons with the method of coupled coherent states. *Phys. Rev. A* **2019,** *100* (1), 013607.
4. Shalashilin, D. V., Zombie states for description of structure and dynamics of multi-electron systems. *Journal of Chemical Physics* **2018,** *148* (19), 194109.

Wavepacket dynamics at conical intersection and its spectroscopic manifestation

Lipeng Chen

Max Planck Institute for the Physics of Complex Systems, 01187, Dresden, Germany
Email: lchen@pks.mpg.de



In the past decades we have seen impressive progresses on the computational study of the ultrafast nonadiabatic dynamics at conical intersections. Yet, the molecular wavepacket dynamics at conical intersection has not been directly characterized and monitored via femtosecond nonlinear spectroscopy. We have combined the hierarchy equation of motion, the multiple Davydov ansatz, the Multiconfigurational Ehrenfest dynamics, and the trajectory surface hopping method with the nonlinear response function formalism to simulate four-wave-mixing (4WM) signals for a set of conical intersection systems. Our results show that the signals indeed visualize evolutions of the wave packet at conical intersections, and these evolutions reveal key features of the photoinduced dynamics, such as electronic/nuclear populations, electronic/nuclear coherences, and electronic/nuclear energy transfer processes.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 29
Time: Dec 9, 2021 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/96269184597?pwd=M0hpaDYvZVJJMjM0QjlSajUwQ3NQZz09

Meeting ID: 962 6918 4597
Passcode: 792635
One tap mobile
+16465588656,,96269184597#,,,,*792635# US (New York)
+13126266799,,96269184597#,,,,*792635# US (Chicago)

Dial by your location
- +1 646 558 8656 US (New York)
- +1 312 626 6799 US (Chicago)
- +1 301 715 8592 US (Washington DC)
- +1 253 215 8782 US (Tacoma)
- +1 346 248 7799 US (Houston)
- +1 669 900 9128 US (San Jose)

Meeting ID: 962 6918 4597
Passcode: 792635
Find your local number: https://buffalo.zoom.us/u/aeHoFEY8ri

Join by SIP
96269184597@zoomcrc.com

Join by H.323
162.255.37.11 (US West)
162.255.36.11 (US East)
115.114.131.7 (India Mumbai)
115.114.115.7 (India Hyderabad)
213.19.144.110 (Amsterdam Netherlands)
213.244.140.110 (Germany)
103.122.166.55 (Australia Sydney)
103.122.167.55 (Australia Melbourne)
149.137.40.110 (Singapore)
64.211.144.160 (Brazil)
69.174.57.160 (Canada Toronto)
65.39.152.160 (Canada Vancouver)
207.226.132.110 (Japan Tokyo)
149.137.24.110 (Japan Osaka)
Meeting ID: 962 6918 4597
Passcode: 792635