

VISTA Seminar

Seminar 36

April 27, 2022

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

TOC:

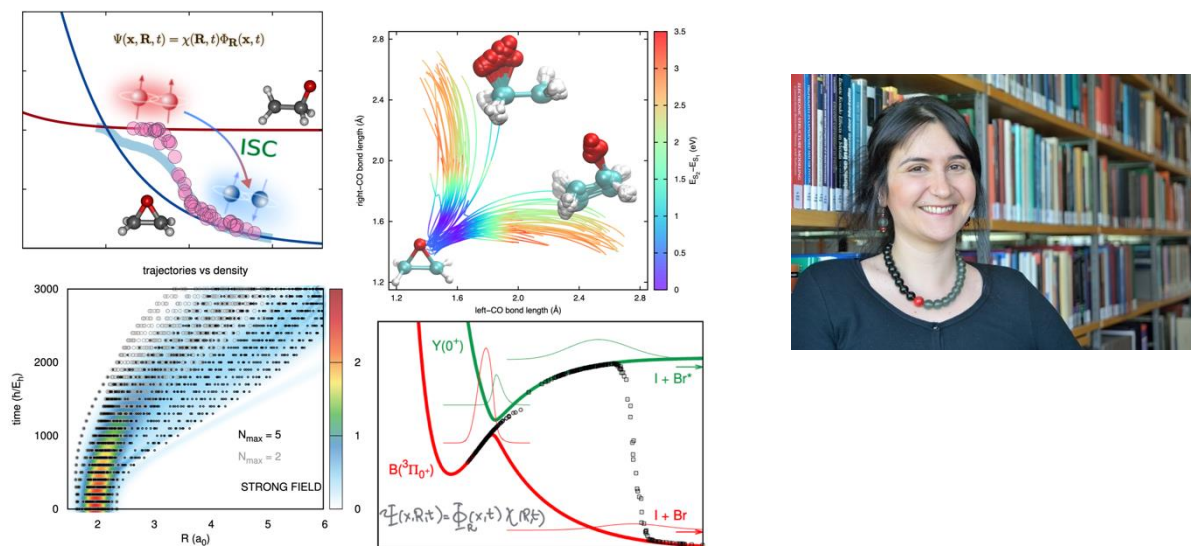
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Theory and simulation of ultrafast processes in molecules with the exact factorization

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In this talk I will review the theoretical basis of the exact factorization of the electron-nuclear wavefunction [1] to describe excited-state dynamics in molecules. I will focus on two main aspects of the theory, one related to the perspective offered by the exact factorization in comparison to the usual Born-Huang representation [2,3], and one related to the development of trajectory-based algorithms for nonadiabatic dynamics. More specifically, I will apply the coupled-trajectory mixed quantum-classical (CT-MQC) algorithm [4] and its recently-proposed combination with the trajectory surface hopping idea [5] to the simulation of various ultrafast processes, such as photoisomerization processes [6-8] or light-driven nonadiabatic dynamics [9].

References:

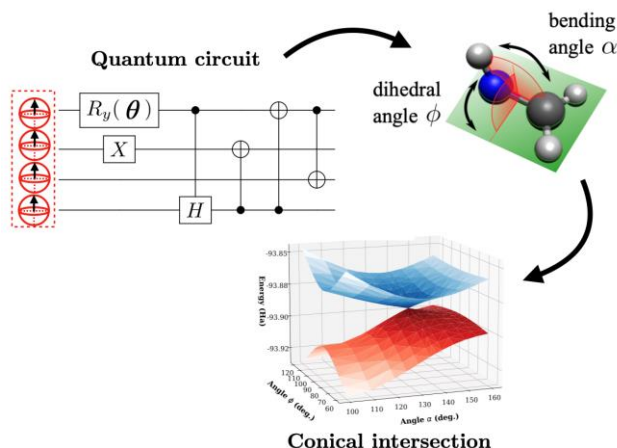
- [1] A. Abedi, N. T. Maitra, E. K. U. Gross, *Phys. Rev. Lett.* (2010).
- [2] F. Agostini, B. F. E. Curchod, *WIREs Comput. Mol. Sci.*, 9, e1417 (2019).
- [3] L. M. Ibele, B. F. E. Curchod, F. Agostini, *J. Phys. Chem. A*, 126, 1263—1281 (2022).
- [4] S. K. Min, F. Agostini, E. K. U. Gross, *Phys. Rev. Lett.*, 115, 073001 (2015).
- [5] C. Pieroni, F. Agostini, *J. Chem. Theory Comput.*, 17, 5969—5991 (2020).
- [6] S. K. Min, F. Agostini, I. Tavernelli, E. K. U. Gross, *J. Phys. Chem. Lett.*, 8, 3048—3055 (2017).
- [7] E. Marsili, M. Olivucci, D. Lauvergnat, F. Agostini, *J. Chem. Theory Comput.*, 10, 6032—6048 (2020).
- [8] F. Talotta, S. Morisset, N. Rougeau, D. Lauvergnat, F. Agostini, *Phys. Rev. Lett.*, 124, 033001 (2020).
- [9] M. Schirò, F. G. Eich, F. Agostini, *J. Chem. Phys.*, 154, 114101, (2021).

Quantum computing for quantum chemistry

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In quantum computing, solving the electronic structure problem is considered as the “killer application” for near term quantum computers. To treat this problem, a great focus has been paid to the development of hybrid-classical-quantum algorithms such as the well-known “Variational-Quantum-Eigensolver” (VQE). While VQE has been proficiently applied to find electronic eigenstates/energies of various small molecules, using this approach on more complex systems is still a genuine challenge especially when peculiar spectral features such as conical intersections are present. In nature, conical intersections play a key role in many prominent reactions. For instance, in the process of vision: the retinal molecule is known to undergo a photoisomerisation mediated by a non-radiative relaxation through a conical intersection. In such a situation, characterizing the phenomenon requires to precisely describe the shape of the conical intersection, with both qualitative and quantitative high-level treatments. This makes it a difficult target to current quantum algorithms, such as VQE.

Motivated by this problem, I recently introduced a new quantum algorithm called the “State-Averaged Orbital-Optimized VQE” (SA-OO-VQE) [1] designed to treat on an equal footing degenerate states on near term quantum computers. In this talk, I will introduce the theory of SA-OO-VQE and illustrate how it works on the description of the conical intersection of a prototype molecule. Furthermore, I will introduce new extensions to the algorithm recently developed to estimate nuclear gradients and non-adiabatic couplings.

References:

- [1] Yalouz, Saad, et al. "A state-averaged orbital-optimized hybrid quantum–classical algorithm for a democratic description of ground and excited states." *Quantum Science and Technology* 6.2 (2021).
- [2] Yalouz, Saad, et al. "Analytical nonadiabatic couplings and gradients within the state-averaged orbital-optimized variational quantum eigensolver." *Journal of Chemical Theory and Computation* (2022).

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 36

Time: Apr 27, 2022 10:00 AM Eastern Time (US and Canada)

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