VISTA Seminar

Seminar 12

9:30 – 11:00 am EST / 2:30 – 4:00 pm GMT / 3:30 pm – 5:00 pm Paris

TOC:

Quantum dynamics with the quantum trajectory-guided adaptable Gaussian bases

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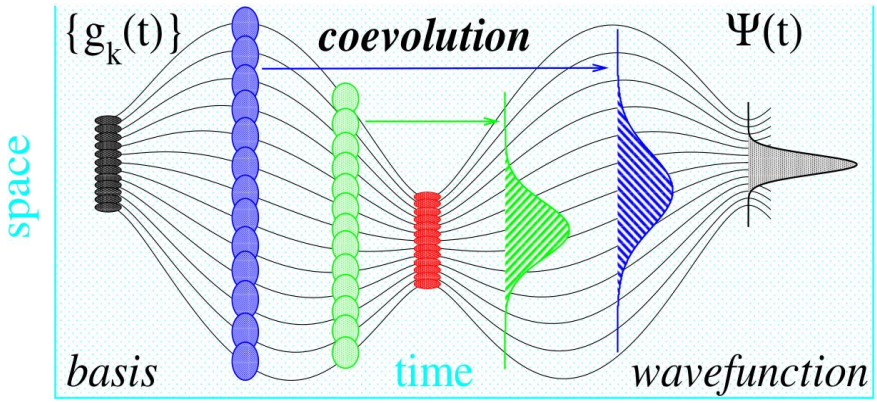

The computational cost of describing a general quantum system fully coupled by anharmonic interactions scales exponentially with the system size. Thus, an efficient ba sis representation of wave functions is essential, and when it comes to the large-amplitude motion of high-dimensional systems, the dynamic bases of Gaussian functions are often employed. The time dependence of such bases is determined from the variational principle or from classical dynamics; the former is challenging in implementation due to singular matrices, while the latter may not cover the configuration space relevant to quantum dynamics. Here we describe a method using Quantum Trajectory-guided Adaptable Gaussian (QTAG) bases [1,2] "tuned" including the basis position, phase, and width to the wave function evolution, thanks to the continuity of the probability density along the quantum trajectories defined by the de Broglie-Bohm formulation of the Schrodinger equation [3]. Thus, an efficient basis in configuration space is generated, bypassing the variational equations on the parameters of the Gaussians. We also propose a time propagator with basis transformation by projections which lends efficiency and stability to the QTAG dynamics. The method is demonstrated on benchmark and chemical models, including the ammonia inversion dynamics, and the double-well dynamics in high-dimensions.

References:

[1] Bing Gu, and Sophya Garashchuk. Quantum Dynamics with Gaussian Bases Defined by the Quantum Trajectories. J. Phys. Chem. A 120, 3023–3031 (2016).

[2] Matthew Dutra, Sachith Wickramasinghe, and Sophya Garashchuk. Quantum Dynamics with the Quantum Trajectory-Guided Adaptable Gaussian Bases. Journal of Chemical Theory and Computation 16, 18-34 (2020). DOI: 10.1021/acs.jctc.9b00844

[3] Sophya Garashchuk, Jacek Jakowski & Vitaly A. Rassolov. Approximate quantum trajectory dynamics for reactive processes in condensed phase. Molecular Simulation 41:1-3, 86-106 (2015). DOI: 10.1080/08927022.2014.907493

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

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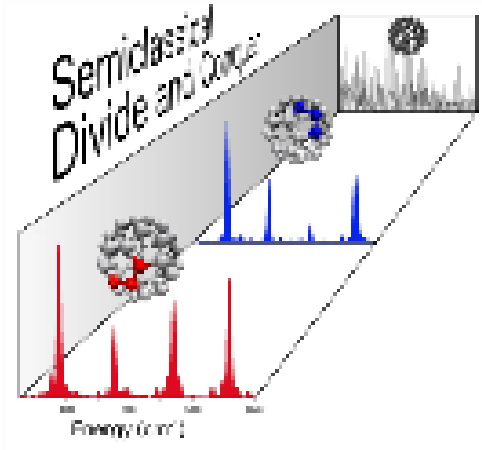
Semiclassical dynamics has long been known to be able to calculate accurately vibrational power spectra of small, isolated molecules with inclusion of quantum effects like zero-point energies, overtones, and quantum resonances.[1,2] Recent methodological advances have permitted application of semiclassical 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.

References:

[1] A.L. Kaledin, W.H. Miller, *J. Chem. Phys.* **118**, 7174 (2003).
[2] W.H. Miller, *Proc. Natl. Acad. Sci. U.S.A.* **102**, 6660 (2005).
[3] M. Ceotto, G. Di Liberto, R. Conte, *Phys. Rev. Lett.* **119**, 010401 (2017).
[4] M. Micciarelli, R. Conte, J. Suarez, M. Ceotto, *J. Chem. Phys.* **149**, 064115 (2018).
[5] C. Aieta, M. Micciarelli, G. Bertaina, M. Ceotto, *Nat. Commun.* **11**, 4348 (2020).
[6] A. Rognoni, R. Conte, M. Ceotto, *Chem. Sci.* advance article (2021). DOI: 10.1039/D0SC05785A
[7] F. Gabas, R. Conte, M. Ceotto, *J. Chem. Theory Comput.* **13**, 2378 (2017).
[8] F. Gabas, G. Di Liberto, R. Conte, M. Ceotto, *Chem. Sci.* **9**, 7894 (2018).
[9] R. Conte, P.L. Houston, C. Qu, J. Li, J.M. Bowman, *J. Chem. Phys.* **153**, 244301 (2020).
[10] F. Gabas, R. Conte, M. Ceotto, *J. Chem. Theory Comput.* **16**, 3476 (2020).

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