VISTA Seminar

Seminar 57

October 11, 2023

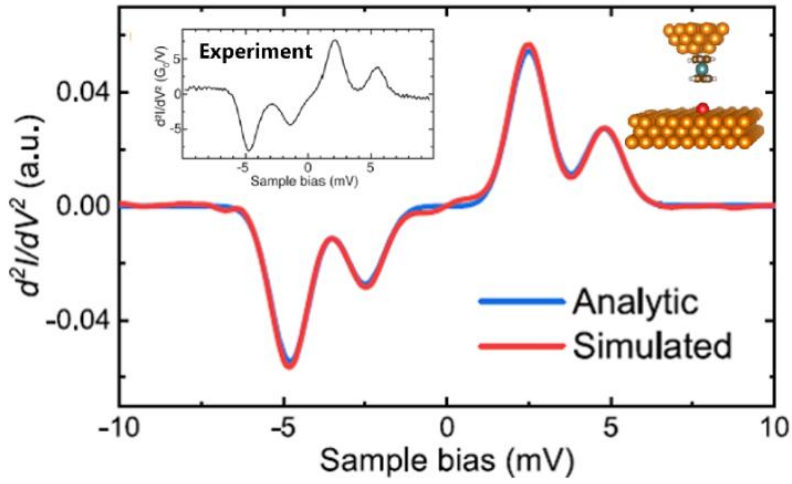
10:00 am – 11:30 am EST / 3:00 – 4:30 pm GMT London / 4:00 pm – 5:30 pm CET Paris / 10 pm CST Beijing

TOC:

Quantum dissipative dynamics approach to many-body open quantum systems

Xiao Zheng

Department of Chemistry, Fudan University, Shanghai 200433, PR China
Email: xzheng@fudan.edu.cn



Open quantum systems have found widespread applications in physics, chemistry, and biology. The dissipative couplings between these systems and their surrounding environments have a profound impact on their dynamic and thermodynamic properties. However, an accurate and universal description of open quantum systems is challenging, especially when dealing with systems that experience fluctuations in particle number, non-Markovian memory effects, or strong many-body correlations. To address these challenges, our research efforts over the past decade have been focused on developing innovative theoretical methods. In this presentation, I will discuss some of our recent progress, which include the development of the fermionic hierarchical equations of motion (HEOM) and stochastic equation of motion (SEOM) methods [1-2]. These methods have proven to be practical and useful tools, as demonstrated through simulations on single molecular junctions that are precisely measured and controlled using scanning tunneling microscopy [3-5]. Additionally, these methods have allowed us to unravel the intricate interplay between low-energy spin excitations and Kondo correlations.

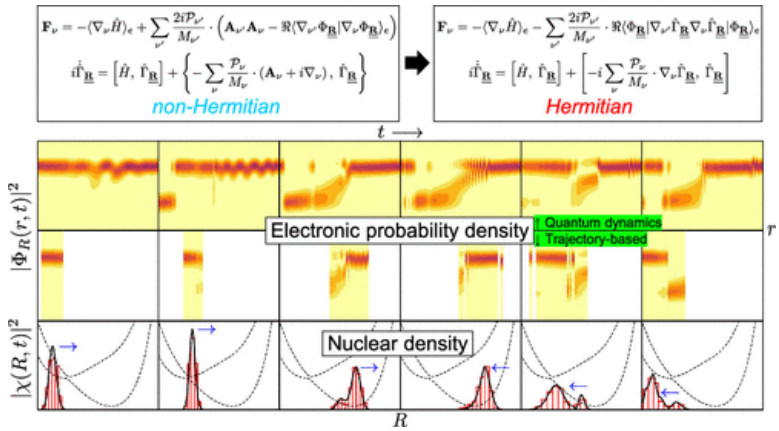
References:

[1] D. Zhang, L. Zuo, L. Ye, Z.-H. Chen, Y. Wang, R.-X. Xu, X. Zheng, and Y. J. Yan, *J. Chem. Phys.* 158, 014106 (2023).
[2] L. Han, V. Chernyak, Y.-A. Yan, X. Zheng, and Y. J. Yan, *Phys. Rev. Lett.* 123, 050601 (2019).
[3] X. Li, L. Zhu, B. Li, J. Li, P. Gao, L. Yang, A. Zhao, Y. Luo, J. Hou, X. Zheng, B. Wang, and J. Yang, *Nat. Commun.* 11, 2566 (2020).
[4] L. Zuo, Q. Zhuang, L. Ye, Y. J. Yan, and X. Zheng, *J. Phys. Chem. Lett.* 13, 11262 (2022).
[5] B. Verlhac, N. Bachellier, L. Garnier, M. Ormaza, P. Abufager, R. Robles, M.-L. Bocquet, M. Ternes, N. Lorente, and L. Limot, *Science* 366, 623 (2019).

Electron-nuclear correlation to the realtime time-dependent density functional theory from mixed-quantum classical equations based on the exact factorization

Daeho Han

Department of Chemistry, School of Natural Science, Ulsan National Institute of Science and Technology (UNIST), S. Korea; Email: dhhan4869@gmail.com



Among various decoherence-based nonadiabatic molecular dynamics methods, those based on exact factorization (XF) have proven useful. The mixed quantum classical (MQC) equations derived from XF contain non-Hermitian electron-nuclear correlation terms, due to the complexity of the original electron-nuclear coupling within XF. By introducing a density matrix representation to the MQC equations, we found new Hermitian-type equations that guarantee equivalent time evolution. The Hermiticity of the equations enables a stable correlated dynamics for the Shin-Metiu model, using a straightforward Crank-Nicolson propagator. Furthermore, we deduced a time-dependent Kohn-Sham (TDKS) analog from the XF-based density matrix representation. Using this modified realtime time-dependent density functional theory (RT-TDDFT) approach, we developed a novel nonadiabatic method named orbital-based surface hopping dynamics through XF (OSHXF). The OSHXF method successfully described the dynamics of an excited ethylene molecule, suggesting the potential for applying XF-based decoherence to more extended systems within RT-TDDFT.

References

Han, D.; Ha, J.-K.; Min, S.K. “Real-Space and Real-Time Propagation for Correlated Electron–Nuclear Dynamics Based on Exact Factorization.” *J. Chem. Theory Comput.*, **2023**, 19, 8, 2186-2197.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 57
Time: Oct 11, 2023 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/98236646491?pwd=OCswQ0FDMjhBTzZvME1nZEhKYnI1UT09

Meeting ID: 982 3664 6491
Passcode: 138136