VISTA Seminar

Seminar 35

April 13, 2022

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

TOC:

Nonadiabatic Dynamics, Machine Learning and Time-Resolved Pump-Probe Spectra

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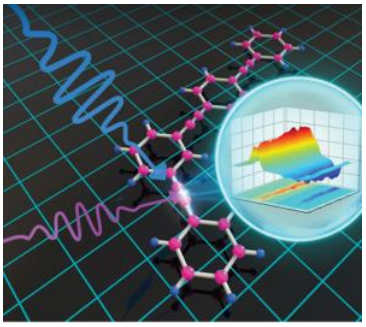

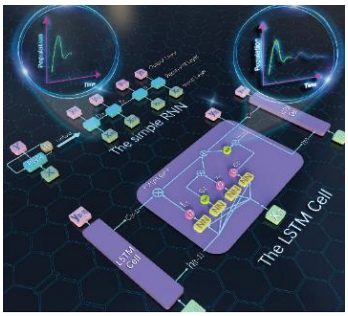

Nonadiabatic dynamics widely exist in photophysics, photochemistry and photobiology. We tried to develop theoretical approaches to study the photoinduced nonadiabatic dynamics. Two topics will be discussed.

1. We combined the doorway-window representation of the nonlinear response theories and ab initio nonadiabatic dynamics to simulate the time-resolved pump-probe spectra. Two interesting examples, including the photoinduced excited-state energy transfer and the nonadiabatic photoisimerization, are discussed.
2. We tried to combine deep leaning method and numerical accurate quantum dynamics approach to simulate the long-time quantum evolution of open quantum system. This approach allows us to obtain the evolution of reduced density matrix of open quantum system with a low computational cost. It demonstrates that the deep learning approach is the important tool to speed up the long-time quantum evolution.

References:

1. C. Xu; K. Lin; D. Hu; F. L. Gu; M. F. Gelin; Z. Lan,. J. Phys. Chem. Lett., 13, 661-668 (2022).
2. K. Lin, J. Peng, F. L. Gu, Z. Lan. J. Phys. Chem. Lett., 12, 10225-10234 (2021).
3. D. Hu, J. Peng, L. Chen, M. F. Gelin, Z. Lan. J. Phys. Chem. Lett., 12, 9710-9719 (2021)

Diagrammatic quantum Monte Carlo toward the calculation of transport properties in disordered semiconductors

Yu-Chen Wang and Yi Zhao

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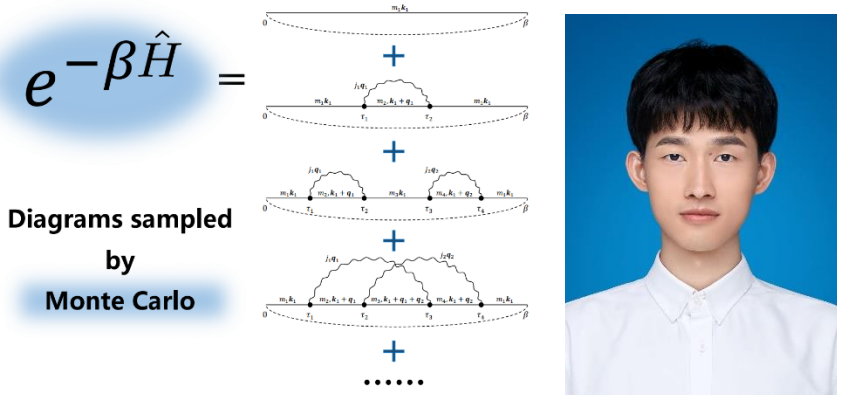

Structural disorders at the microscopic level generally exist in materials such as semiconductors and light-harvesting systems. These disorders may substantially alter the electronic structure of the system and ulteriorly influence the transport properties of the carriers (electron, hole, or exciton) therein. The complex interplay between disorders and electronic couplings often leads to unexpected and sometimes exhilarating phenomena such as the band-like mobilities in high-mobility organic semiconductors and the formation of the small polaron in many metallic oxide semiconductors, the accurate description of which challenges the currently available theoretical methods.

In this report, I will introduce a newly developed diagrammatic quantum Monte Carlo approach which is able to deal with the imaginary time propagator involving both dynamic disorder (i.e., electron-phonon interactions) and static disorder of local or nonlocal nature in a unified and numerically exact way. The establishment of the whole framework relies on a general reciprocal-space expression and a generalized Wick's theorem for the static disorder. The numerical cost of this approach is independent of the system size, and various physical quantities such as the thermally averaged coherence, Matsubara one-particle Green's function and current autocorrelation function can be efficiently evaluated in the thermodynamic limit (infinite in the system size). By combining with proper numerical analytic continuation methods and first-principles calculations, this approach can be used to accurately calculate various transport properties in realistic semiconductors involving multiple electronic energy bands, high-frequency optical and low-frequency acoustic phonons, different forms of dynamic and static disorders, anisotropy, etc.

Reference

[1] Wang, Y.-C. and Zhao, Y. Diagrammatic quantum Monte Carlo toward the calculation of transport properties in disordered semiconductors. 2022, arXiv:2203.12480.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 35
Time: Apr 13, 2022 10:00 AM Eastern Time (US and Canada)

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