VISTA Seminar

Seminar 22

August 18, 2021

9:30 – 11:00 am EDT / 1:30 – 3:00 pm GMT / 3:30 pm – 5:00 pm Paris

TOC:

Energy flow in quantum systems

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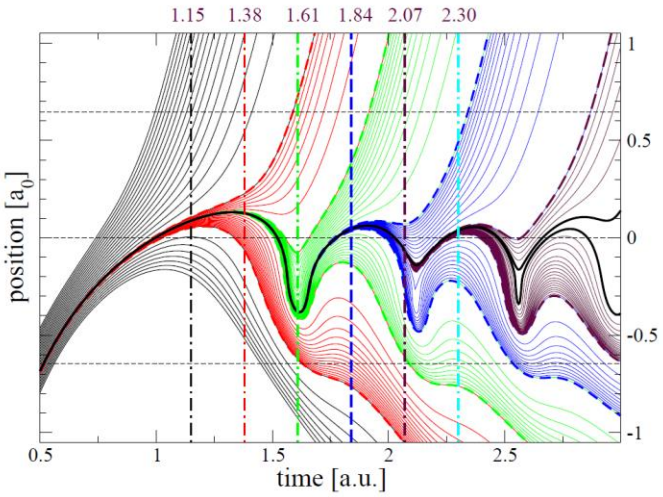

The Madelung-de Broglie-Bohm formulation of the Schrodinger equation casts the time-evolution of a wavefunction as dynamics of an ensemble of quantum, or Bohmian, trajectories, interacting via the non-local quantum potential. This trajectory perspective gives insight into the quantumness (or classicality) of a given system due to clear partitioning of the energy into classical and quantum components. In this presentation we introduce a local system-independent measure of the quantumness of dynamics, based on the energy time-change ('quantum power') in coordinate space. Based on applications to model chemical systems, we argue that during the transition from the quantum to classical regime, defined as compression of quantization, the quantum features in dynamics do not 'disappear' but are pushed back in time. This feature may be used to gauge the validity of the semiclassical and other approximate Gaussian-based dynamics approaches in applications to anharmonic systems. Application of the proposed measure to the interference and the tunneling models reveal unexpected features of quantum dynamics. In particular, we demonstrate the origins of the computational complexity in the deep tunneling dynamics. We also discuss the quantum-classical transitions using 2D harmonic Kohen-Tully model.

Benchmarking the Surface Hopping method to include nuclear quantum effects

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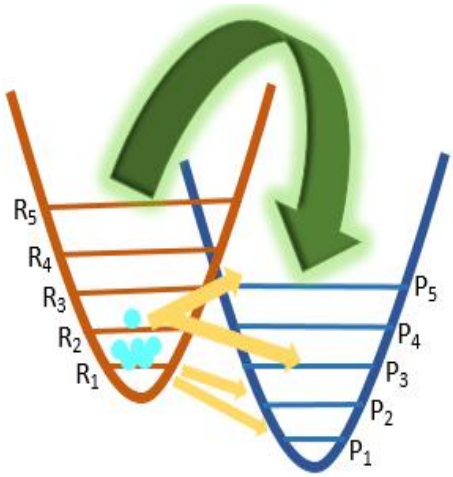

The fewest switches surface hopping (FSSH) method is a popular algorithm used for simulating non-adiabatic dynamics. There have been several applications where it can be applied, like proton and electron transfer, photo-excited state dynamics, etc. In the present work, we have benchmarked the surface hopping method for the spin-Boson model Hamiltonian for such a case where both electronic and vibrational non-adiabaticity is essential to define the dynamics. We have considered the parameters for the spin-Boson model such that the system lies in a deep tunneling regime. Two kinds of simulations have been done for all sets of parameters. First is treating one bath mode as quantum mechanical and the other to treat it classically. The rates obtained from the former were compared with Fermi's golden rule answer and that of later compared with the Marcus rate. Also, the thermal population obtained from FSSH was compared with the Boltzmann answer. Further, we have looked into the different versions of decoherence schemes in Augmented-FSSH and compared the velocity reversal schemes in case of frustrated hopes. Finally, we have proposed a rate theory to analyze the failure of surface hopping in for some particular set of parameters.

With this benchmarking of the FSSH method, we are all set to apply the same on a molecule (FMO) within the spin-Boson Hamiltonian. We have reached on some preliminary conclusions for the FMO parameters.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 22
Time: Aug 18, 2021 09:30 AM Eastern Time (US and Canada)

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