Exploring the exact factorization adapted nonadiabatic dynamics on various potential landscapes

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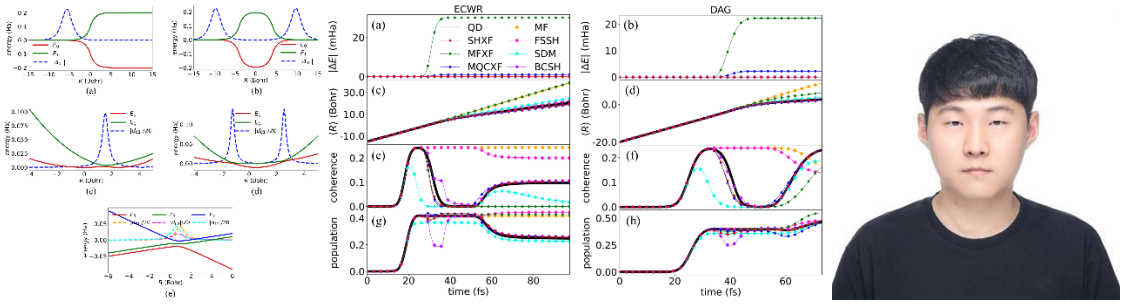

While the decoherence-corrected nonadiabatic dynamics methods based on exact factorization (XF) have proven useful for simulating excited-state phenomena, it is still lacking to assess these methods among a pool of pre-existing nonadiabatic methods with various potential landscapes. In this presentation, I will explain brief ideas of the independent-trajectory XF methods–SHXF, MQCXF and MFXF, i.e., the surface hopping, mixed quantum-classical and mean-field variation based on XF and explore their dynamics on a variety of 1D model Hamiltonians. Compared to the conventional methods including the Ehrenfest, fewest-switches surface hopping (FSSH), simple decay of mixing (SDM) and branching-corrected surface hopping (BCSH), their behaviors and performance are analyzed systematically based on the exact discrete-variable representation (DVR) dynamics.

Reference

Han, D.; Akimov, A. V. Nonadiabatic Dynamics with Exact Factorization: Implementation and Assessment. *J. Chem. Theory Comput.* **2024**, 20 (12), 5022–5042.