Landau-Zener surface hopping algorithm for nonadiabatic dynamics in photoinduced reactions

Weiwei Xie
Institute of Physical Chemistry (IPC), Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Trajectory surface hopping (TSH) methods have been widely used in the nonadiabatic dynamics simulations for photoinduced reactions. In this computational method, classical trajectories are allowed to hop stochastically between adiabatic surfaces, governed by the comparison of a computed transition probability with a random number. Perhaps the most popular way to evaluate the transition probability is based on fewest switches (FS) ansatz [1], in which the hopping probability is assumed to be proportional to the flux of electronic population. In this talk, I will introduce an alternative method, namely, Landau-Zener surface hopping (LZSH) [2], in which the hopping probability is evaluated by Landau-Zener formula. First, I will discuss the accuracy of FSSH and LZSH in comparison with exact quantum dynamics calculations for two presentative examples, the nonadiabatic photodissociation of phenol [3] and ultrafast internal conversion of pyrazine [4]. In both cases, we show that LZSH and FSSH with decoherence correction can reasonably reproduce population transfer dynamics including the vibrationally driven electronic population oscillations. The second part of my talk will focus on the application of the LZSH approach to the study of the mechanism of photoinduced water splitting reaction [5].

References

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