

Time-dependent Adaptive Sampling Configuration Interaction

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Describing electron dynamics in presence of strong electron correlation is a challenging methodological problem. In this work, we have attempted to develop such methods both with a time-independent and external-field driven time-dependent Hamiltonian. With the time-independent Hamiltonian, we can evaluate various auto-correlation functions, for example, dipole-dipole type. On the other hand, with the time-dependent Hamiltonian, we can study charge migration in presence of ultrashort pulses, for example. We will present numerical studies of both kinds. For the correlated method, we have considered a selected CI method, namely Adaptive Sampling Configuration Interaction (ASCI) as implemented in Q-Chem []. All the current developments are made in Q-Chem as well.