Real-time TDHF/TDDFT calculation with efficient time evolution

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Electron dynamics, which is an ultrafast phenomenon occurring in femtoseconds, was recently observed by experiments and has attracted much attention. To theoretically describe electron dynamics, we can use real-time propagation (RT) method of time-dependent theories, such as the time-dependent Hartree-Fock (TDHF) method and the time-dependent density functional theory (TDDFT). However, the RT-TDHF/TDDFT calculations[1-3] have limited applications than the conventional frequency-domain TDHF/TDDFT for evaluating excitation spectra and frequency-dependent polarizabilities, because evaluation of the time evolution operator is computationally demanding. The Chebyshev expansion technique in real space[4,5] is one of the efficient methods for evaluation of the time evolution operator. This method has been applied to time-dependent Schrödinger equation for nuclear wave packet dynamics and succeeded in decreasing computational cost. In this study, we applied this Chebyshev expansion method to RT-TDHF calculation to achieve efficient time evolution.

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