

Time-dependent generalized-active-space configuration-interaction approach to photoionization dynamics of atoms and molecules

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We present a time-dependent theory to investigate electron dynamics and photoionization processes of atoms and diatomic molecules interacting with strong laser fields including electron-electron correlation effects. We compare the recently formulated time-dependent generalized-active-space configuration interaction (TD-GASCI) theory [1, 2] with the Multiconfiguration time-dependent Hartree-Fock method. The TD-GASCI method is applied to strong field ionization of LiH in 3D with short laser pulses [3]. We give a detailed comparison between fully converged TD-GASCI simulations and approximations thereof. Finally, we apply it to high harmonic generation in helium where the ionization step is initiated by a XUV pulse [4]. Excellent agreement between the TD-GASCI simulations and the experimental results is achieved.

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