Abstract Submitted
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Excitation ionization of atoms and diatoms as a test of the all-active-electron MCTDHF method[1] DANIEL HAXTON, KEITH LAWLER, C. WILLIAM MCCURDY, Chemical Sciences, Lawrence Berkeley National Lab — We have developed an implementation of the Multiconfiguration Time-Dependent Hartree-Fock (MCTDHF) method [PRA 83, 063416 (2011)]. MCTDHF is an adaptive method for solving the time-dependent Schrodinger equation and we apply it to atoms and diatoms in ultrafast laser pulses. The method is built to describe nonlinear phenomena and incorporates both an all-active-electron representation and the ability to include diatomic nuclear motion without the Born-Oppenheimer approximation. As a diagnostic of the method, we have calculated photoionization cross sections for: valence ionization of Beryllium, and of HF, LiH, and N2 in the fixed nuclei approximation; 1s ionization of Beryllium; and dissociative ionization of H2+ including nuclear motion with full nonadiabatic coupling. We will present results that demonstrate the convergence of the method with respect to the number of time-dependent orbitals and discuss the prospects of the method for describing nonlinear phenomena.

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