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Nonperturbative calculation of multidimensional spectra using the Multiconfiguration Time-Dependent Hartree Fock method ZACHARY WALTERS, C. WILLIAM MCCURDY, University of California, Davis and Lawrence Berkeley National Lab — A nonperturbative approach to multidimensional spectroscopy is demonstrated which makes use of a recent implementation of the Multiconfiguration Time-Dependent Hartree Fock (MCTDHF) method to describe the correlated many-electron response of atoms and molecules to VUV or X-ray pulses. A multidimensional spectrum, for example a three pulse photon echo spectrum, is determined by the dipole polarization $\mathbf{P}(\mathbf{t}) = \langle \mathbf{\Psi}(\mathbf{t}) | \hat{\mu} | \mathbf{\Psi}(\mathbf{t}) \rangle$ of the system following a series of ultrafast laser pulses. Phase matched components of the polarization can be found using established techniques by calculating polarization corresponding to pulse sequences which vary only in their carrier envelope phases, then solving a linear system of equations for the phase matched components. An atomic test case making use of subfemtosecond VUV pulses is presented.

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