Multi-Configuration Time-Dependent Hartree-Fock theory applied to quantum dots CARLOS DESTEFANI, ALEXANDER PEGARKOV, CHRIS MCDONALD, THOMAS BRABEC, University of Ottawa, PAWEL HAWRYLAK, Institute for Microstructural Sciences, NRC — The Multi-Configuration Time-Dependent Hartree-Fock method (MCTDHF) is a tool that can be used to study the electron dynamics of several multielectronic systems under strong laser fields. It is based on a variational principle applied to the time-dependent Schrodinger equation, where the many-particle ansatz wavefunction is a sum over configurations, with both coefficients and single-particle functions being time-dependent and optimized at each time step. In this way, electron correlation is taken into account and a faster convergence within a smaller expansion is obtained when compared to other mean-field theories. This method yields two sets of coupled non-linear differential equations to be solved by a certain integration scheme. These so-called working equations are propagated from a given initial state, yielding the wavefunction under the influence of the external field and allowing the study of the multielectronic dynamics under the laser pulse. As a first application of the MCTDHF theory, we analyze the multielectronic dynamics of isolated and coupled harmonic gated quantum dots driven by an intense laser field.

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