Title:	Electronic quntum dynamics of molecules in string laser fields: novel algorithms and novel effects
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Abstract:	Attosecond light-matter interaction is a developing area in the eld of strong laser-matter inter- action. With attosecond spectroscopy, the motion of electrons in atoms and molecules and can be observed along with the long term e ects in molecular vibration due to the driven electrons. In last decade, there has been signi cant experimental advancement in the generation of attosecond pulses. For an adequate theoretical and computational description of the strong eld e ects in molecules, the time-dependent solution for a driven many-body system is essential, in spite of the conceptual, numerical and computational di culties involved. The thesis then goes on to a description of the (t; t0)-method for quantum dynamics with general time-dependent Hamiltonians in the context of laser-atom, laser-molecule interactions. The evolution operator for the (t; t0)-method requires a huge storage space with a large operation count for the propagation. The analytical block diagonalization of the Floquet Hamiltonian is proposed for the evolution of the time-dependent Hamiltonian. This combination of the split operator method with the block-diagonalization technique of the chosen order is approximate the full evolution operator. The number of operations are drastically reduced using new algorithm. Hence, only matrices of the order of the number of position basis functions need to be stored. Thus, the presented algorithm is an e ective tool for solving the (t; t0; t00) problem for interactions with a bi-chromatic laser, di erent symmetries of laser elds, and a single-frequency laser pulse with explicit interactions of the pulse envelope. Following up on the (t; t0) implementation, the dynamics of two electrons in a three-dimensional symmetric double-well has been shown as a test case. In the presence of the laser, a paired up barrier-top state of electrons is formed, with the oscillating eld overcoming the increased electron repulsion. A switching o of the laser induces ionization,thus giving a temporal control over the process. The main feature of the thesis is the development of a (t; t0) formalism for real-time Hartree-Fock electronic dynamics of molecules at xed geometries, in high-intensity laser elds. The novelty of the method lies in the ease of incorporation of memory e ects in the dynamics by encoding the explicit time-dependence of the mean- eld two-particle operator into the e ective Hamiltonian. A memory- e ect is built in, by learning from the frequency-dependent Fourier components of the charge-density bond-order matrix, extracted via a windowed Fourier transform. In comparison to an instantaneous representation of the time-dependence of the two-particle operator, our method results in a backward time propagation with minimal error for large time steps. The algorithm is presented together with several test cases dihydrogen, water, acetylene, ethylene and benzene in a high intensity laser pulse, using standard Gaussian basis sets, with the calculation of several time-dependent properties. A general set of conclusions and future perspectives of all the work is then presented together with the beginnings of a package for electronic dynamics named ABELDYN.
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