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Ab initio calculations of correlated electron dynamics in ultrashort pulses[1]

JOHANNES FEIST, ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA and Institute of Theoretical Physics, TU Vienna, Austria

The availability of ultrashort and intense light pulses on the femtosecond and attosecond timescale promises to allow to directly probe and control electron dynamics on their natural timescale. A crucial ingredient to understanding the dynamics in many-electron systems is the influence of electron correlation, induced by the interelectronic repulsion. In order to study electron correlation in ultrafast processes, we have implemented an ab initio simulation of the two-electron dynamics in helium atoms. We solve the time-dependent Schrödinger equation in its full dimensionality, with one temporal and five spatial degrees of freedom in linearly polarized laser fields. In our computational approach, the wave function is represented through a combination of time-dependent close coupling with the finite element discrete variable representation, while time propagation is performed using an Arnoldi-Lanczos approximation with adaptive step size. This approach is optimized to allow for efficient parallelization of the program and has been shown to scale linearly using up to 1800 processor cores for typical problem sizes. This has allowed us to perform highly accurate and well- converged computations for the interaction of ultrashort laser pulses with He. I will present some recent results on using attosecond and femtosecond pulses to probe and control the temporal structure of the ionization process. This work was performed in collaboration with Stefan Nagele, Renate Pazourek, Andreas Kaltenbäck, Emil Persson, Barry I. Schneider, Lee A. Collins, and Joachim Burgdörfer.

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