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Exterior complex scaling method in TDDFT calculations: MPI and HHG of Ar atoms[1] DMITRY A. TELNOV, KSENIA E. SOSNOVA, EFIM B. ROZENBAUM, St. Petersburg State University, Russia, SHIH-I CHU, University of Kansas — Exterior complex scaling (ECS) method is applied in the framework of time-dependent density functional theory (TDDFT) to study multiphoton ionization (MPI) and high-order harmonic generation (HHG) of multielectron atoms in intense laser fields. ECS allows to impose correct (outgoing-wave) boundary conditions on the wave functions at large distances. In our implementation, ECS is combined with the time-dependent generalized pseudospectral method (GPS) for accurate and efficient solution of time-dependent Kohn-Sham equations. We make use of LB94 exchange-correlation potential which proved accurate in calculations of unperturbed electronic structure of Ar. Calculations of MPI and HHG are performed for the laser pulses with the wavelength 800 nm and several peak intensities. HHG spectrum exhibits an intensity-independent minimum corresponding to the photon energy of about 50 eV which is closely related to the Cooper minimum observed in photoionization cross section of Ar. We found that results obtained with the frozen-core potential (that is, not including dynamic response of the electron density to the laser field) significantly overestimate MPI probabilities as compared with those calculated by TDDFT.

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