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Breakup of the H_2 molecule by xuv laser pulses: A time-dependent treatment in prolate spheroidal coordinates[1] XIAOXU GUAN, KLAUS BARTSCHAT, Drake University, BARRY I. SCHNEIDER, National Science Foundation — We report calculations of the triple-differential cross section for one-photon double ionization of molecular hydrogen, based on a fully *ab initio*, nonperturbative approach to solve the time-dependent Schrödinger equation in prolate spheroidal coordinates. The spatial coordinates ξ and η are discretized in a finite-element discrete-variable representation. The wave packet of the laser-driven two-electron system is propagated in time through an effective short iterative Lanczos method. For both symmetric and asymmetric energy sharing, the present results agree to a satisfactory level with most earlier predictions for the absolute magnitude and the shape of the angular distributions, except for the recent time-independent calculations based on the exterior complex scaling method in prolate spheroidal coordinates [1]. Extensive tests of the numerical implementation were performed, including the effect of truncating the Neumann expansion for the dielectronic interaction on the description of the initial bound state and the predicted cross sections.

[1] L. Tao, C. W. McCurdy, and T. N. Rescigno, Phys. Rev. A **82** (2010) 023423.

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