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Effect of moving nuclei in multiphoton ionization of the H_2^+ ion[1]

XIAOXU GUAN, KLAUS BARTSCHAT, Drake University, BARRY I. SCHNEIDER, National Science Foundation — We propose an accurate *ab initio* numerical method to depict the dynamics of the nuclear fragments and the entangled motion of the nuclei and the electron in the laser-driven H_2^+ ion. Building on recent work [1], we solve the time-dependent Schrödinger equation in prolate spheroidal coordinates and extract the angle-differential cross section for the photoelectron as well as the kinetic energy release spectra of the nuclei. Assuming that the nuclei are frozen in their lowest rotational state, the nuclear coordinate in the wave function is discretized through a finite-element discrete-variable representation (FE-DVR), which is coupled to other FE-DVRs for the electron coordinate. The present procedure in full dimensionality allows us to go beyond the popular fixed-nuclei approximation, the two-channel approximation, and reduced-dimensional models. As a specific example, we discuss the effect of the nuclear motion in the H_2^+ ion followed by two- and three-photon absorption, both in the parallel and perpendicular geometries.

[1] X. Guan, E. Secor, K. Bartschat, and B. I. Schneider, Phys. Rev. A **84** (2011) 032420.

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