Two-photon double ionization of molecular hydrogen in the direct regime

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We have studied the process of direct two-photon double ionization of molecular hydrogen [1]. The fragmentation of the diatomic target following a two-photon impact is a correlated process and the Coulomb repulsion between the electrons is a prerequisite for this process to occur in the direct regime. Understanding the role of electron-electron correlation in the simplest molecular systems could pave the way for further understanding of multi-photon multiple ionization of more complex atomic and molecular targets. In our calculations, the molecular system is treated in the frozen nuclei approximation, which reduces the complexity of the problem to two electrons and a fixed diatomic potential where the nuclei are separated by the equilibrium distance R_0 = 1.4 a.u. The electronic problem is handled in full dimensionality by solving the time-dependent Schrödinger equation for the H_2 molecule interacting with a linearly polarized laser pulse in the XUV regime. We use a laser pulse with a sine-squared carrier envelope and a peak intensity of 10^{13}W/cm^2, lasting for 15 optical cycles of illumination. A series of simulations have been performed, varying the photon energy in the direct regime, $E_\gamma = 26$ eV to $E_\gamma = 33$ eV. Both the orientations have been considered, where the alignment between the polarization of the electromagnetic field and the internuclear axis is parallel and perpendicular. In order to extract information about the double-ionized wave packet, we project the final wave function onto a set of product states of H_2^+ eigenstates with positive energies and as such, neglecting the Coulomb repulsion only in the final state. We extract the total (generalized) cross section for the process in both the geometries and present the results together with the predictions from a simplified model [2], c.f., Figure 1. Results from previous calculations, at the photon energy E_γ =30 eV, are shown for comparison [3,4,5].

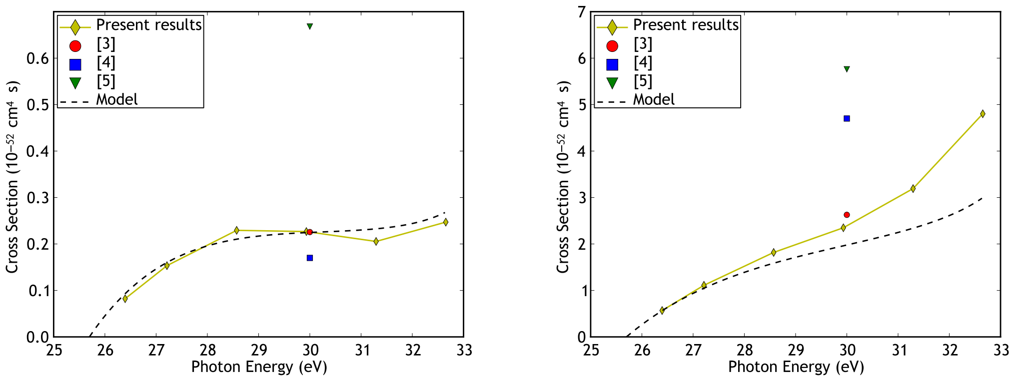

Figure 1: The total (generalized) cross section for the process of direct two-photon double ionization of H_2. The left panel shows the cross section when the polarization direction of the laser pulse is parallel with respect to the internuclear axis. The right panel displays the perpendicular case. The results obtained when solving the full problem are shown as golden diamonds whereas the simplified model predictions are illustrated as a dashed black curve.

References:
[1] A. S. Simonsen, S. A. Sørngård, R. Nepstad, and M. Førre, Phys. Rev. A **85**, 063404 (2012).
[2] M. Førre, S. Selstø, and R. Nepstad, Phys. Rev. Lett. **105**, 163001 (2010).
[3] X. Guan, K. Bartschat, and B. I. Schneider, Phys. Rev. A **84**, 033403 (2011).
[4] J. Colgan, M. S. Pindzola, and F. Robicheaux, J. Phys. B **41**, 121002 (2008).
[5] F. Morales, private communication (2011).