Dissociation and dissociative ionization of H_2^+ in an intense laser field using the time-dependent surface flux method

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Recently, the time-dependent surface flux (t-SURFF) method [1,2] was introduced to extract fully differential ionization spectra of one and two-electron systems from numerical TDSE calculations using minimal simulation volumes.

Here, we show that the t-SURFF method can be extended to obtain spectra for dissociation and dissociative ionization of H_2^+. By dividing the simulation volume into proper spatial regions as shown in Fig.1 (a), the dissociation and dissociative ionization spectra can be obtained by counting the probability flux going through the surfaces. The results for dissociative ionization agree well with [3].

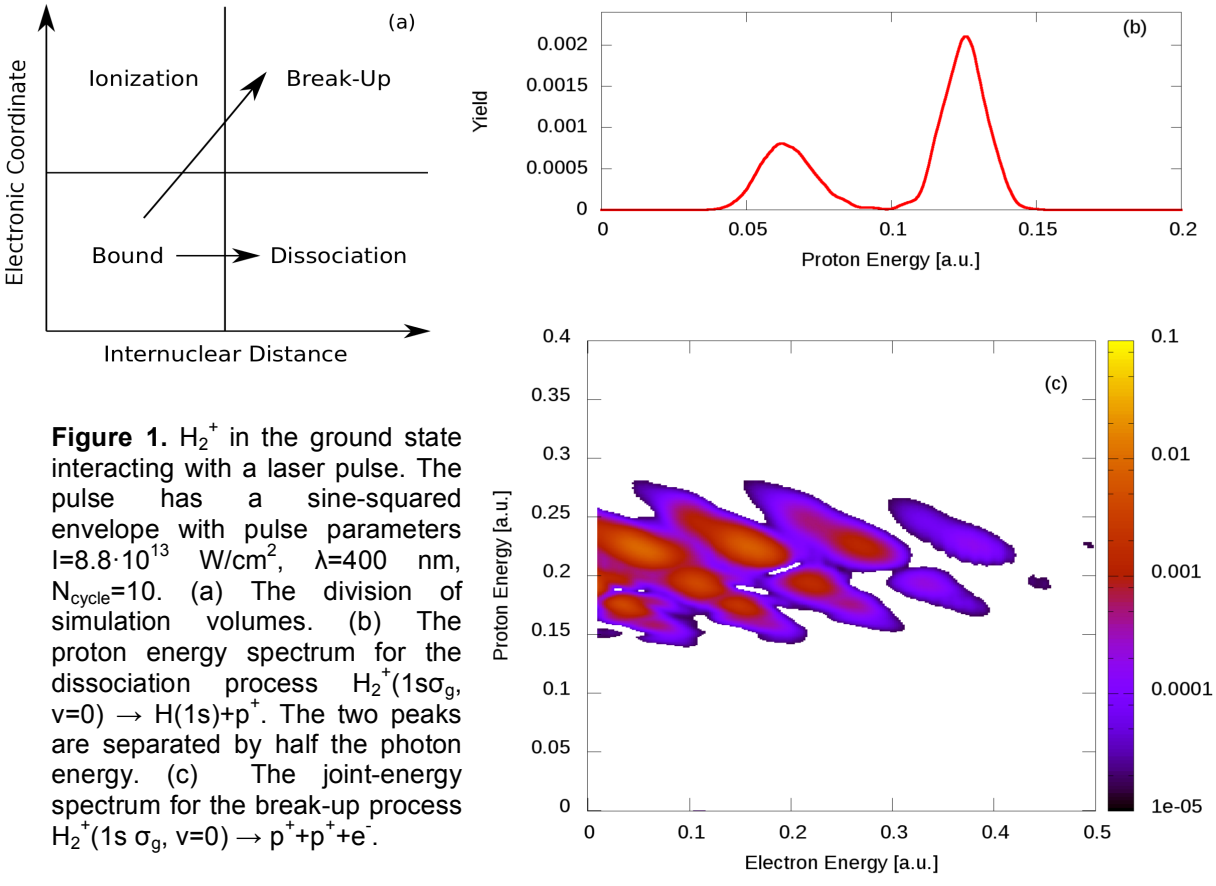

Figure 1. H_2^+ in the ground state interacting with a laser pulse. The pulse has a sine-squared envelope with pulse parameters $I=8.8\cdot10^{13}$ W/cm^2, λ=400 nm, N_{cycle}=10. (a) The division of simulation volumes. (b) The proton energy spectrum for the dissociation process $H_2^+(1s\sigma_g, v=0) \rightarrow H(1s)+p^+$. The two peaks are separated by half the photon energy. (c) The joint-energy spectrum for the break-up process $H_2^+(1s\,\sigma_g, v=0) \rightarrow p^+ + p^+ + e^-$.

References:
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