Strong-field dynamics of a one-dimensional H_2^+/H_2 model molecule

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Synopsis We investigate the dynamics of one-dimensional (1D) H_2^+ and H_2 model molecules in a strong laser field. In the case of H_2^+ we produce momentum distributions to compare with state-of-the-art experiments that resolve the kinetic energy release (KER) spectra. For H_2 our main objective is to study the validity of various approximations, employed in three-dimensional (3D) calculations, by comparing our full 1D model to the 1D analogs of such approximations.

Technological advances have enabled experimentalists to measure 3D momentum distribution of both electrons and ions for ionization of molecules by short instense laser pulses. It remains a challenge, however, to perform theoretical calculations for ionization of even the simplest molecule, H_2^+. Despite several results on the solution of the time-dependent Schrödinger equation (TDSE) within reduced dimensionality models, the calculation of physical observables such as energy or momentum distributions has rarely been accomplished. To address this point, we resolve the previously presented [1] total energy spectra (Fig. 1) by calculating accurate momentum distributions for $p + p + e$.

To investigate the dynamics of H_2^+ in a strong laser field, we use a 1D model with a soft-core Coulomb interaction between the charged particles. We take the soft-core to be a function of the internuclear distance, so that the model system reproduces the true ground state Born-Oppenheimer (BO) potential curve. By comparing our results for dissociation to full 3D calculations, we can estimate to what extent the parametrized soft-core potential actually provides an improvement over the usual 1D model Coulomb potential with fixed soft-core parameters.

For the treatment of H_2, approximations such as the BO approximation, reduced dimensionality for the electrons and the single-active-electron approximation are tested. By generalizing our parametrized soft-core potential to the case of H_2 [2], we will investigate the validity of the various approximate treatments of ionization of H_2 in 3D by comparing the 1D analogs with our full 1D H_2 solution. Also, the restriction to 1D allows us to include all electronic and nuclear degrees of freedom, and, thus, to study the interplay between vibrational motion and single or double ionization.

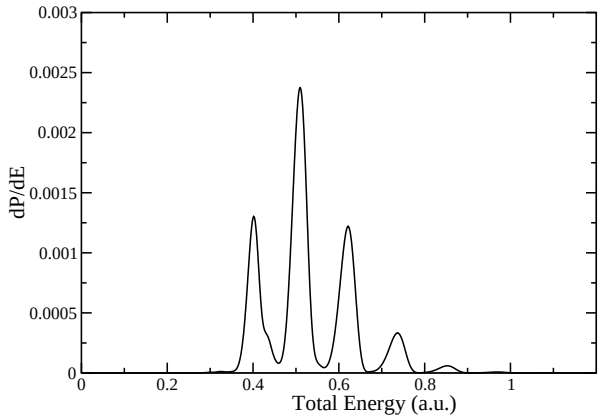

Fig. 1. The total ionization probability for H_2^+ as a function of the total energy (electron plus nuclei) for a 400 nm, 5 fs laser with peak intensity 10^{14} W/cm^2.

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References

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