Nuclear kinetic energy spectra of D2+ in intense laser field: Beyond Born Oppenheimer approximation

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Abstract

The time dependent Schrödinger equation of the aligned deuterium molecular ion numerically is solved for the simulation of the complicated dissociative ionization process and compared with the related experimental results.

Keywords: time-dependent Schrödinger equation, dissociation, ionization, intense laser.

Numerical solution of the TDSE and discussion

In this study, ionization of the H2+ (D2+) under intense linearly polarized pulse of laser fields is simulated by direct solution of the full dimensional electronic TDSE equation, beyond BOA. Time dependent Schrödinger equation in the cylindrical polar coordinate system for H2+ (D2+) molecular ion located in the laser field of $E(t) = E_0 f(t) \cos(\omega t)$ parallel to the $z$ axis (inter-nuclear axis) in atomic unit ($\hbar = m_e = e = 1$) is solved. More details of our calculations were described in our report [3-4].

The main purposes of this article is comparing the simulation results with the results of the recent experimental researches [1-2]. The experimental researches that up until now to be directly started with H2+ and D2+ molecular ion are extremely few. Most experiments were performed using H2 and D2 molecules and during the rise of the laser femtosecond laser pulse (40–140 fs), H2+ (D2+) molecular ion are created. These pulses are usually focused to peak intensities of $\sim 1013–1015$ W/cm2 into the gas jet of unaligned H2 or D2 neutral molecules. When H2 (D2) molecule exposed to a linearly polarized intense femtosecond laser pulse, during the rise of the laser pulse, the first electron is ejected. We assume that this first electron is ejected nearly instantaneously at the time $t_{\text{on}}$ via tunneling. We suppose this process prepares a nuclear wave packet identical to the initial vibrational state of H2 (D2) via a vertical Franck-Condon
transition onto the H2+ ground \( \sigma_g \) state \([1-2]\). In addition, we assume that at the time of the ejection of the first electron, H2 (D2) molecule (and then H2+ (D2+)) is aligned with the linearly polarized intense femtosecond laser pulse. During the remaining part of the laser field envelope, the complicated dissociation-ionization processes of H2+ (D2+) take place and a main aim of this work is exact simulation of these processes. It was discovered theoretically, but with BO approximation, the H2+ molecular ion exhibits a critical distance \( R_c \) at which the molecular ionization rate exceeds the atomic rate by several order of magnitudes and propose that the last electron is ejected mainly at much larger internuclear distances than the equilibrium internuclear separation. It is surprising to investigate about enhanced ionization (EI) and critical distance beyond BO approximation, and study direct relation between EI and kinetic energy release (KER) of nuclear energy. In the following, we investigate these subjects for the D2+.

In this work, we exposed D2+ to femtosecond laser pulses with the different FWHM duration (\( \tau = 40 \) and 140fs). The intensities of both these femtosecond laser pulses are equal to 1.0x10^{14} \text{ W cm}^{-2} \) but their wavelengths are different and equal to 800 and 1200nm respectively. In these simulation, these femtosecond laser pulses turn on suddenly two cycles before the peak of the laser pulse envelop and the simulation begin just at this moment. The nuclear kinetic energy release (KER) of this molecular ion in these intense short laser fields are showed in Fig. 1 [4]. The results of this simulation (black lines) are compared with the experimental results (dotted lines) \([1-2]\) and theoretical calculation with SC approximation (grey lines) \([1-2]\).

![Fig. 1: The kinetic energy release spectrum of nuclear energy of D2+ exposed to femtosecond laser pulses.](image)

**Conclusion**

In conclusion, the electronic full dimensional TDSE numerically solved for the
simulation of the complicated simultaneously dissociative ionization process of one dimensional nuclear dynamics of the D2+. The results of these simulations were compared with the related experimental and other theoretical results. It appears that the electronic full dimensional TDSE without any SC approximation give good agreement with the experimental results.

References