

# Strong-Field Modulated Diffraction Effects in the Correlated Electron-Nuclear Motion in Dissociating $\text{H}_2^+$

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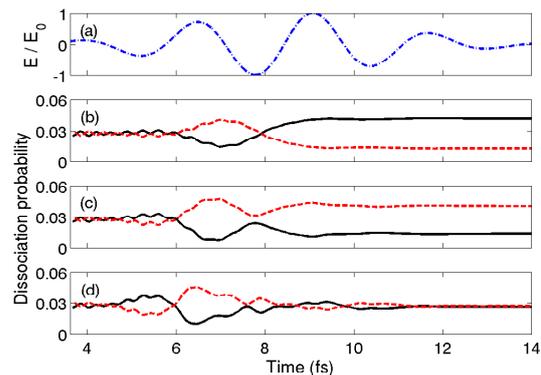
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**Synopsis** : By solving the time dependent Schrödinger equation for  $\text{H}_2^+$  in a pump-probe numerical experiment, we found that the electronic motion can follow or oppose the laser electric force. Our results show that the internal electron dynamics in  $\text{H}_2^+$  is determined by both, the external laser field and intra-molecular electron diffraction.

Current sub-fs laser technology allows for the control of the final localization of the electron in a dissociating hydrogen molecular ion [1, 2]. However, the complex dynamics of the active electron in the time-dependent fields of both nuclei and external laser pulse(s) *before* the electron is localized on one of the nuclei by the rising interatomic barrier is not understood in detail. One may expect that the electron dynamics in the dissociating molecule is an interplay of, at least, field-induced and structural (i.e., interference) effects. We solved the time-dependent Schrödinger equation in three dimensions, and found that the direction of the electronic motion inside the dissociating  $\text{H}_2^+$  can follow or oppose the external laser electric field, depending on the laser intensity [3].

Our model describes a 2-cycle (FWHM), 106 nm,  $10^{13}$  W/cm<sup>2</sup>, Gaussian attosecond pump pulse that excites a dissociating nuclear wave packet on the  $2p\sigma_u$  electronic potential curve of  $\text{H}_2^+$ . A time-delayed infrared laser pulse (2 cycles, 800 nm) is introduced to manipulate the wave function. Fig. 1 shows the evolution of the electronic probability density towards one of the nuclei. For all laser intensities the electron at first oscillates between the two nuclei, as one would expect classically. During the second half of the laser field, the increasing interatomic barrier starts to hinder electron transfer between the nuclei [2], and the electron eventually localizes near one of the protons. Details of the electronic motion are strongly intensity dependent and yield electron localization on opposite centers at different laser peak intensities. For example, the comparison of Figs.1 (b) and (c) near 5.5 fs shows that the electron is moving along either the negative (b) or the positive  $z$ -axis (c), even though the laser profiles are the same. This surprising result shows that the expected electronic motion does not necessarily follow the di-

rection of the laser field. By increasing the intensity further, to  $10^{14}$  W/cm<sup>2</sup>, the electron-transfer dynamics again changes dramatically (d).



**Fig. 1.** (color online) IR laser electric field for a time delay of 5.8 fs (a). Dissociation probability  $P_-(t)$  (solid line) and  $P_+(t)$  (dashed line) for the electron to remain in the  $z < 0$  and  $z > 0$  half space, respectively, for IR laser intensities of  $3 \times 10^{12}$  (b),  $2 \times 10^{13}$  (c), and  $10^{14}$  W/cm<sup>2</sup> (d).

By analyzing the evolution of the molecular wave function in phase space, the corresponding Wigner distribution indicates the path towards electronic localization in terms of the passage of electronic flux through diffraction-induced “momentum gates” that may or may not allow the electron to transfer to the other nucleus [3]. It reveals that the IR laser field dynamically shifts the gates, causing the electron to explore different gates at different laser intensities.

## References

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- [2] F.He, C.Ruiz, and A.Becker, *Phys. Rev. Lett.* **99**, 083002 (2007)
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