Electron Localization and Multiple Ionization Bursts in H_2^+ within a Half Cycle of Near-Infrared Laser Light

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Synopsis We found by numerical simulations that H_2^+ irradiated by intense near-infrared laser light shows multiple bursts of ionization current within a half cycle of the electric field oscillation, in contrast to the intuition given by the quasi-static tunneling ionization picture. We attribute the origin of the multiple bursts to the dynamical localization of the electron at one of the nuclei on the sub-laser-cycle time-scale. A relation between the timing of the bursts and the vector potential of the laser light is derived analytically based on a perturbative solution of a two-state model.

In the traditional picture of quasi-static tunneling ionization of atoms and molecules by intense laser light, ionization events are expected to take place predominantly once per half laser-cycle at the peaks of the electric field. In contrast, our numerical simulations for H_2^+ indicate that there can be multiple bursts of ionization current in a half laser-cycle. Fig. 1 exemplifies the results of our numerical simulations and a two-state analysis for H_2^+ exposed to a laser pulse ($\sin^2$-envelope, 5-cycle FWHM, wavelength 1064 nm, peak intensity 6×10^{13} W/cm^2). Fig. 1(a) shows the laser electric field and vector potential as a function of time over one cycle at the peak intensity, and Fig. 1(d) shows, in the same time window, the time-evolution of the electron density obtained by numerically solving the time-dependent Schrödinger equation for a 1D model of H_2^+ (internuclear distance fixed at 7 a.u.). In Fig. 1(d), one can clearly see multiple ionization packets per half cycle. In Fig. 1(c), we absorbed the outgoing wavepackets to separate the bound electron dynamics from rescattering. From this result, we can deduce that there are two major ionization bursts per half cycle in the present case, and that they are induced by localization of the bound wavepacket at one of the two nuclei.

We have further analyzed the bound electron dynamics using a two-state model with the ground ($|\mathrm{g}\rangle$) and first-excited ($|\mathrm{u}\rangle$) electronic states of H_2^+. Floquet solutions of this system can be obtained using a perturbation method at the limit of strong interaction between the two states [1], and the general solution $|\Psi(t)\rangle$ can be expressed as a superposition of these Floquet states. We derived analytical expressions for the local populations, $(1/2)|(\langle \mathrm{g}| \pm \langle \mathrm{u}|)|\Psi(t)\rangle|^2$, which are plotted in Fig. 1(b) as a function of time, and identified that their extrema are at the time instants $\{t_n\}$ defined by $A(t_n) = \tilde{A} - (n\pi - \chi)/(2d_{\mathrm{gu}})$, where n is an integer, $A(t)$ and $\tilde{A}$ are the vector potential and its time-average, respectively, d_{gu} is the dipole matrix element between $|\mathrm{g}\rangle$ and $|\mathrm{u}\rangle$, and χ is an angle determined by the superposition coefficients of the Floquet states. Grid lines in Fig. 1(a,b) indicate $\{t_n\}$ and $\{A(t_n)\}$. The electron localization observed in Fig. 1(c) is well reproduced by the two-state model in Fig. 1(b), and, therefore, the timing of the ionization bursts can be predicted as the localization maxima of the simple analytical model.

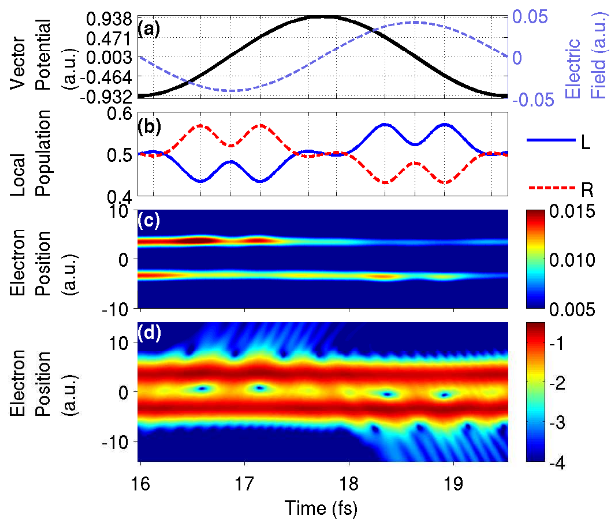

Fig. 1. Results of numerical simulations and a two-state analysis for H_2^+ are shown for one laser-cycle at the peak of a 5-cycle-FWHM pulse.

References

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