Probing electron localization in laser-driven diatomic molecules by attosecond pulses

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Synopsis We explore the possibility of using attosecond pulses to probe electronic dynamics of molecules driven by a laser field in real time. Taking advantage of the interference in the photoionization process, we show that the information of the electronic dynamics, particularly the electron localization can be imaged with attosecond pulses. We expect the same technique can be used to imaging atoms or molecules polarized by laser fields.

Different from imaging electron localization of a freely evolving molecules with attosecond pulses [1, 2], we consider in this work the possibility of probing the laser-driven electronic dynamics of a model H_2^+ molecule initially in the ground state. The electron is driven oscillating in the two charge-resonance states (HOMO and LUMO orbitals) by a laser field of frequency larger than the transition energy. The dynamics is essentially following the oscillation of the laser field. With H_2^+ pre-aligned in space, 2D simulations are performed with the IR laser field and the probing attosecond pulse parallel and perpendicular to the molecular axis respectively.

In order to image the dynamics occurring within one optical cycle, we numerically calculated the photoelectron momentum spectra by applying an attosecond pulse with photon energy of 90 eV and FWHM duration of 100 as. We find that the photoelectron spectrum is streaked strongly by the laser field, even though no direct ionization is induced by the laser field. The characterization of the laser field has to be well known to obtain the full information of the molecular state. With that assumed, the spectra can be restored by removing the effect of the laser field on the outgoing electron easily, since the electric field does not vary much within the time of the XUV pulse.

Probing the electron localization, on the other hand, does not require knowing the laser field exactly. The interference pattern of the photoelectron momentum spectra stays the same even after the propagation of the quasi-free electron in the laser field. Therefore the contrast of the maximum to the minimum of electron yields provides the localization information. When the yield at the maximum differs largely from that at the minimum, strong interference is occurring suggesting the electron is nearly equally localized around the two nuclei. When the interference is hardly recognized, the electron is localized in one of the nuclei as shown in Fig. 1.

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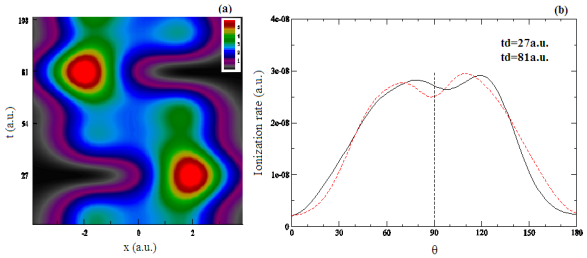

Fig. 1. (a) The variation of electron probability distribution with time and (b) the angle-resolved photonelectron spectra at time delay of 27 a.u.(solid lines) and 81 a.u. (dashed lines) respectively. The laser intensity is 5×10^{13}W/cm2.

References

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