

Extreme ultraviolet (XUV) pulse shaping with aligned molecules

Zhinan Zeng¹, Ruxin Li, Zhizhan Xu

State Key Laboratory of High Field Laser Physics, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai, People's Republic of China 201800

Synopsis: We theoretically propose a simple scheme to shape the xuv pulse on attosecond timescale with the aligned molecule. This may offer a new way to manipulate and control the photon emission on attosecond timescale.

Many experiments, e.g. the tomographic imaging of molecular orbitals, the quantum interference during HHG and the proton dynamics in molecules, have been carried out with the HHG generated by the molecules, e.g. O₂, N₂, CO₂ [1, 2]. With the orientation dependence of the molecular HHG and the field-free alignment of the molecule, we can produce the xuv pulse of different shape just by adjusting the time delay between the laser pulse to induce the nonadiabatic molecular alignment and the laser pulse to generate the HHG.

We use the CO₂ molecule to demonstrate this process numerically. For CO₂ molecule whose valence orbital has even parity symmetry, the valence orbital can be expressed by

$$\Psi_g(\bar{x}) = N[\Phi(\bar{x} + \bar{R}/2) + \Phi(-\bar{x} + \bar{R}/2)] \quad (1)$$

Where N is normalization factors, $\Phi(\bar{x})$ is the atomic orbital, $\bar{R}/2$ and $-\bar{R}/2$ the positions of the nuclei (for CO₂ molecules, the positions of the two O atoms). With the molecular orbital expression and the Lewenstein model [3], we can calculate the molecular dipole moment $d(\theta, t)$ of any orientation in the time domain in which θ is the angle between the polarization of the laser pulse and the axis of the CO₂ molecule.

The laser-induced orientation dynamics of CO₂ can be calculated by solving the time-dependent Schrodinger equation (TDSE) [4], in which the rigid-rotor approximation is used. After solving the TDSE, we can obtain the angular distribution $\rho(\theta, \tau)$ of the molecules, where τ is the delay time after the intensity peak of the laser pulse which induced the orientation dynamics. In the simulation, the pulse intensity is 0.03a.u. ($3.16 \times 10^{13} \text{W/cm}^2$) and the pulse duration is 60fs. The rotational temperature of CO₂ molecules is taken to be 40K.

With $d(\theta, t)$ and $\rho(\theta, \tau)$, we can calculate the delay time dependent dipole moment with expression below,

$$S(\tau, t) = 2\pi \int_0^\pi \rho(\theta, \tau) d(\theta, t) d\theta \quad (2),$$

where τ is the delay time between two laser pulses. Then we can easily calculate the delay time dependent HHG by performing the Fourier-Transform (FT) on the $S(\tau, t)$.

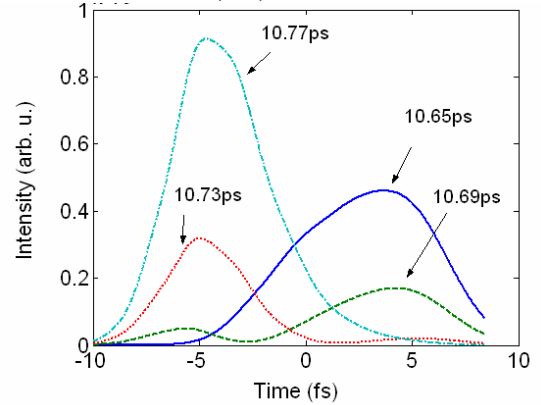


Fig. 1. the temporal profiles of the xuv pulses with different delay time.

In Fig. 1, when the delay time changes from 10.65ps to 10.77ps, the xuv pulse changes from a single-peak pulse to a double-peak pulse. Then right peak of the double-peak pulse becomes weaker and weaker gradually. When the delay time becomes to be 10.77ps, the xuv pulse becomes to be a single-peak pulse again.

In conclusion, we have proposed a simple scheme to shape the temporal profile of the xuv pulse. This result may offer a new way to manipulate and control the photon emission in the xuv domain.

References

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¹Email: zhinan_zeng@mail.siom.ac.cn