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# High-order harmonic generation in polyatomic systems

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**Synopsis** We present a theoretical approach of high-order harmonic generation (HHG) in polyatomic molecules based on the strong-field approximation (SFA) and within the frame of the single electron approximation. Our model allow us to turn on and off contributions having distinct physical origins or corresponding to different physical mechanisms. Results in di- and tri-atomic systems are shown. In addition a time-frequency analysis is presented to investigate the relative weight of the different electron trajectories contributing to the HHG spectra.

High-order harmonic generation (HHG) results from the interaction of a strong field with atomic and molecular systems. It configures one of the main processes used to extract electron structural and dynamical information about the atomic or molecular targets with sub-femtosecond temporal resolution. Moreover, it is the workhorse for the generation of attosecond pulses.

Here we develop an analytical description of HHG, which extends the well established strong-field approximation (SFA) [1]. Our approach involves two innovative aspects: i) first, using a non-local short-range model, but separable potential, we analytically calculate the bound-free and rescattering transition matrix elements for both atomic and molecular multicenter systems. In comparison with the standard approaches for the HHG process, these analytic derivations of the different matrix elements allow us to study directly how the HHG spectra depend on the atomic target and laser-pulse features. We can turn on and off contributions having distinct physical origins or corresponding to different physical mechanisms. In this way we quantify their weights in the various regions of the HHG spectra; ii) second, as Ref. [2, 3] reports, in our theory the multicenter matrix elements are free from non-physical gauge and coordinate system dependent terms – this is achieved by adapting the coordinate system, in which SFA is formulated, to the centre from which the corresponding part of the time dependent wave function originates.

We present results for di- ($H_2$) and tri-atomic ($CO_2$, $H_2O$) molecular systems exposed to a linearly polarized strong laser field. Additionally, our model captures the existence of an interference minima pattern in every molecular harmonic spectra. These minima can be considered as a multiple-slit type interference phenomenon, ubiquitously present in every strong field process involving a multicenter target [4].

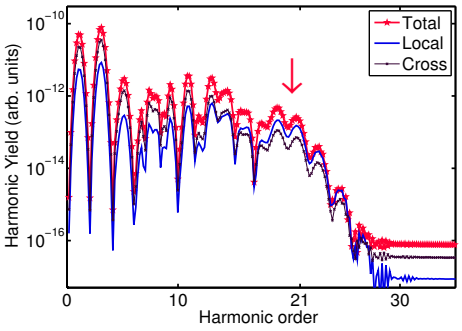


**Figure 1**. Total, Local and Cross contributions to an $H_2O$ HHG spectra (in logarithmic scale) computed using our quasi-classical SFA model. The HHG spectra are computed averaging 8 different molecular orientations.

## References

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