

# Above-threshold ionization processes in diatomic molecules driven by strong laser fields

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**Synopsis** In this work we develop a general theory to study above-threshold ionization (ATI) in symmetric diatomic molecules. It is based on the Strong Field Approximation (SFA) and allows us to underpin different physical processes corresponding to (i) direct tunneling ionization; (ii) electron rescattering on the center of origin; and, finally, (iii) electron rescattering on a different center. Very good agreement is observed in comparison of the results obtained with the time-dependent Schrödinger equation (TDSE). Our model also captures the dependence of the ATI spectra on the internuclear distance making possible to retrieve molecular structural information.

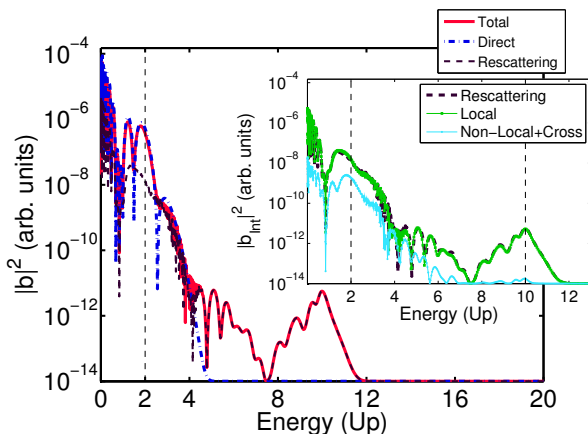
Strong field photoemission and electron recollision provide a viable route to extract electronic and nuclear dynamics from molecular targets with attosecond temporal resolution. However, since an *ab-initio* treatment of even the simplest diatomic systems is beyond today's computational capabilities, approximate qualitative descriptions are warranted.

In this contribution, we develop a theoretical approach to model the photoelectrons resulting from the interaction of an intense laser with molecular targets. We present a general theory for symmetric diatomic molecules in the single active electron approximation that, amongst other capabilities, allows adjusting both the internuclear separation and molecular potential in a direct and simple way. More importantly, we derive an analytic approximate solution of the TDSE, based on a generalized SFA [1, 2].

Using our approach we obtain expressions for the laser-induced electron emission transition amplitudes from each molecular centres, and accelerated then in the strong laser field. In addition, our model directly underpins different underlying physical processes that correspond to i) direct tunnelling ionization; ii) electron rescattering on the centre of origin; iii) and, finally, electron rescattering on a different centre. In Fig. 1 we show results for  $H_2^+$  molecules, obtained using our the modified SFA model.

One innovative aspect of our theory is the fact that the dipole matrix elements are free from non-physical gauge and coordinate system dependent terms – this is achieved by adapting the coordinate system, in which the SFA is performed, to the centre from which the corresponding part of the time dependent wave function originates.

Our analytic results agree very well with results extracted from the TDSE for  $H_2^+$  molecules. Moreover, the theoretical model was applied to describe laser-induced electron diffraction (LIED) measurements of  $O_2^+$  molecules, obtained at ICFO, and reproduces the main features of the experiment very well. Our approach can be extended in a natural way to more complex molecules and multi-electron systems [3].



**Figure 1.** Different contributions to the  $H_2^+$  photoelectron spectra (in logarithmic scale) calculated by using our model. The internuclear distance is set to  $R = 2.6$  a.u. and the laser peak intensity to  $I_0 = 4 \times 10^{14} \text{ W} \cdot \text{cm}^{-2}$ .

## References

- [1] M. Lewenstein *et al.* 1995 *Phys. Rev. A.* **51** 1507
- [2] N. Suárez *et al.* 2015 *Phys. Rev. A.* **92** 063421
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