

## Molecular Resolvent Operator for $\text{H}_2^+$ molecule

R. E. F. Silva<sup>\*1</sup>, F. Catoire<sup>†</sup>, P. Rivière<sup>\*</sup>, H. Bachau<sup>†</sup>, and F. Martín<sup>\*,\*\*</sup>

<sup>\*</sup> Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, Cantoblanco 28049, Madrid, Spain

<sup>†</sup> Centre des Lasers Intenses et Applications CNRS-CEA-Univ. Bordeaux I, 351 Cours de la Libération, Talence F-33405, France

<sup>\*\*</sup> Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nanociencia), Cantoblanco, 28049 Madrid, Spain

**Synopsis** We present a theoretical method to extract photoelectron and nuclear kinetic energy spectra of molecules under intense ultrashort laser pulses. The method is applied to  $\text{H}_2^+$  photoionization and dissociation within a 3D model of the  $\text{H}_2^+$  molecule [1]. This method is an extension to molecules of the resolvent technique originally proposed for atoms [2], which was recently implemented to extract absolute values of photoelectron and nuclear kinetic energy spectra [3, 4].

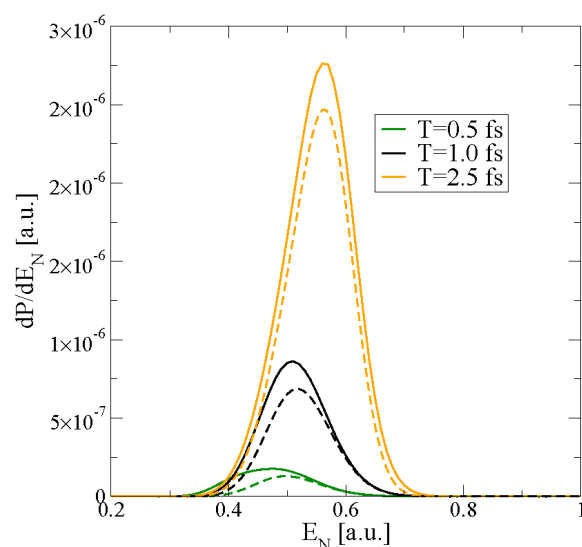
One of the most valuable informations that we can extract from a theoretical solution of the Time-Dependent Schrödinger equation (TDSE) is the spectra of the fragments. In a molecule we can have different fragments and the usually calculated spectra are the photoelectron spectra and the nuclear kinetic energy release. These two spectra can provide more information in a correlated spectra [5]. In this work we have extended the resolvent technique to molecules within a 3D model of the  $\text{H}_2^+$  molecule [1]. To achieve that we propose a factorization of the resolvent operator into an electronic resolvent operator and a nuclear resolvent operator, where the first one selects a given electronic state and the second one extracts the probability associated to a given vibronic energy [4].

$$\hat{R} = \hat{R}_N \hat{R}_{ele} \quad (1)$$

This method allows to extract differential probability densities for the different ionization and dissociation channels in the Born-Oppenheimer approximation.

We have studied the multiphoton ionization of the  $\text{H}_2^+$  molecule with low intensities of the laser field and we are able to obtain fully differential spectra both in nuclear and electronic energy and also angular distributions. With a fully differential spectra we are capable of providing a much more complete description of the dynamics behind photoionization and photodissociation. Our results have been successfully compared with those previously obtained in the lit-

erature [6].



**Figure 1.** KER spectra resulting from a pulse with central frequencies  $\omega = 0.6$  a.u. The pulse duration is indicated in the figure. We have used relatively low intensities ( $10^{12}$  W/cm<sup>2</sup>). We also show the results from Ref. [6] (dashed lines).

### References

- [1] T. Niederhausen, U. Thumm and F. Martín, *Journal of Physics B* **45**, 105602-1 105602-9 (2012).
- [2] K. J. Schafer and K. C. Kulander, *Phys. Rev. A* **42**, 5794 (1990).
- [3] F. Catoire and H. Bachau, *Phys. Rev. A* **85**, 023422 (2012).
- [4] F. Catoire, R. E. F. Silva, P. Rivière, H. Bachau and F. Martín, *Phys. Rev. A* **89**, 023415 (2014).
- [5] R. E. F. Silva, F. Catoire, P. Rivière, H. Bachau and F. Martín, *Phys. Rev. Lett.* **71**, 063405 (2005).
- [6] A. Palacios, S. Barmaki, H. Bachau, and F. Martín, *Phys. Rev. A* **110**, 113001 (2013).

<sup>1</sup>E-mail: [rui.silva@uam.es](mailto:rui.silva@uam.es)

