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

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**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].

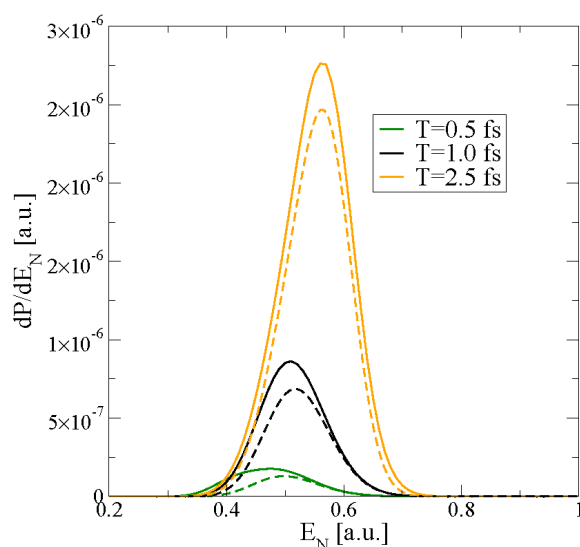
One of the most valuable informations that we can extract from a theoretical solution of the Time-Dependent Schrödinger equation (TDSE) is the spectra of the fragments. In a molecule we can have different fragments and the usually calculated spectra are the photoelectron spectra and the nuclear kinetic 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

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