TIME-DEPENDENT MODEL CALCULATIONS FOR THE MOLECULAR HYDROGEN ION IN A STRONG ULTRA-SHORT LASER PULSE

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We have revisited the problem of a hydrogen molecular ion in the presence of a short intense laser field. Our approach for time-propagation the initial state subject to the Schrödinger equation is similar to that presented by Kulander *et al.* [1]. A common simplification to the full problem is the reduction to one dimension with two degrees of freedom, one for the nuclear separation (R) and one for the electronic motion along the internuclear (z) axis, with the electric field also along this axis. The goals of the present project are: 1) to apply our method, developed for e-H collisional excitation and ionization [2], to an explicitly time-dependent problem; 2) to check different time-propagation schemes; 3) to visualize the results; 4) to extract the physics by projection techniques; and 5) to try avoiding masking potentials that reduce the norm of the wavefunction.

Going beyond the Born-Oppenheimer approximation, we solve the time-dependent Schrödinger equation

$$i\frac{\partial\Psi(R,z,t)}{\partial t} = \left[-\frac{1}{2\mu}\frac{\partial^2}{\partial R^2} - \frac{1}{2}\frac{\partial^2}{\partial z^2} + \frac{1}{\sqrt{R^2+q_n}} - \frac{1}{\sqrt{(z-R/2)^2+q_e}} - \frac{1}{\sqrt{(z+R/2)^2+q_e}} + z f(t) \mathcal{E}_0 \sin(\omega t) \right] \Psi(R,z,t) \quad (1)$$

by time-propagating the initial state

$$\Psi(R,z,t=0) = F_v^{1\sigma_g}(R) G_R^{1\sigma_g}(z), \quad (2)$$

where $G_R^{1\sigma_g}(z)$ is the electronic ground state for fixed R and $F_v^{1\sigma_g}(R)$ is the vibrational state v .

The screening parameters $q_n = 0.03$ and $q_e = 1.0$ are used to smooth out the Coulomb singularity. The term $z f(t) \mathcal{E}_0 \sin(\omega t)$ represents the effect of the electric field with amplitude $\mathcal{E}_0$ and angular frequency ω . Finally, $f(t)$ is a smooth turn-on/turn-off function for the field.

We have used intensities of $1-2 \times 10^{18} \text{ W/m}^2$, turn-on/turn-off times of 2–4 periods, and on-times up to about 20 periods. We also follow the system for several periods after the pulse is over. Typical observables to calculate are $\langle R(t) \rangle$ and $\langle z(t) \rangle$. However, $\langle R(t) \rangle$ has limited meaning since it includes vibration, dissociation, and Coulomb explosion; the same is true for $\langle z(t) \rangle$. Looking at the complete nuclear and electronic distributions reveals significantly more information.

We therefore created movies to watch for bond-stretching and bond-healing, vibrational excitation, dissociation (electron stays with one of the protons) and ionization (electron leaves the system and protons undergo “Coulomb explosion”). Links to these movies can be found at <http://bartschat.drake.edu/>. We are currently working on our projection techniques to find, for example, the probability of exciting a particular vibrational and/or electronic state.

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References

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- [2] K. Bartschat, S. Riordan and G. Ver Steeg, Phys. Rev. A **65** (2002) 060701(R).