TIME-DEPENDENT MODEL CALCULATIONS FOR H_2^+ IN A STRONG ULTRA-SHORT LASER PULSE

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OVERVIEW:

I. **Time Propagation of the Schrödinger Equation**

II. **Visualization**

III. **Extracting Physics**

IV. **Conclusions and Outlook**

Model for H_2^+ in a Strong Laser Field

- The basic idea was presented by Kulander *et al.*, Phys. Rev. A 53 (1996) 2562.
- Many other groups have worked on this and similar problems.
- A common simplification of 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.
- Goals of the present project :
  - Apply our method, developed for e–H collisional excitation and ionization, to an explicitly time-dependent problem
  - Check a different time-propagation scheme (leap-frog)
  - Visualization of the results
  - Extract physics by projection techniques
  - Try to avoid masking potentials that reduce the norm of the wavefunction

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

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

by time-propagating the initial state

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

- Here $G_R^{1\sigma_g}(z)$ is the electronic ground state for fixed R.
- $F_v^{1\sigma_g}(R)$ is a vibrational level for the nuclear motion. [We show results for $v=0$, but can take arbitrary distributions.]
- 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 $1-2\times 10^{18}$ W/m^2, turn-on/turn-off times of 2–4 periods, and on-times of about 10 periods.
- We also follow the system for several periods after the pulse is over.

Extracting Physics

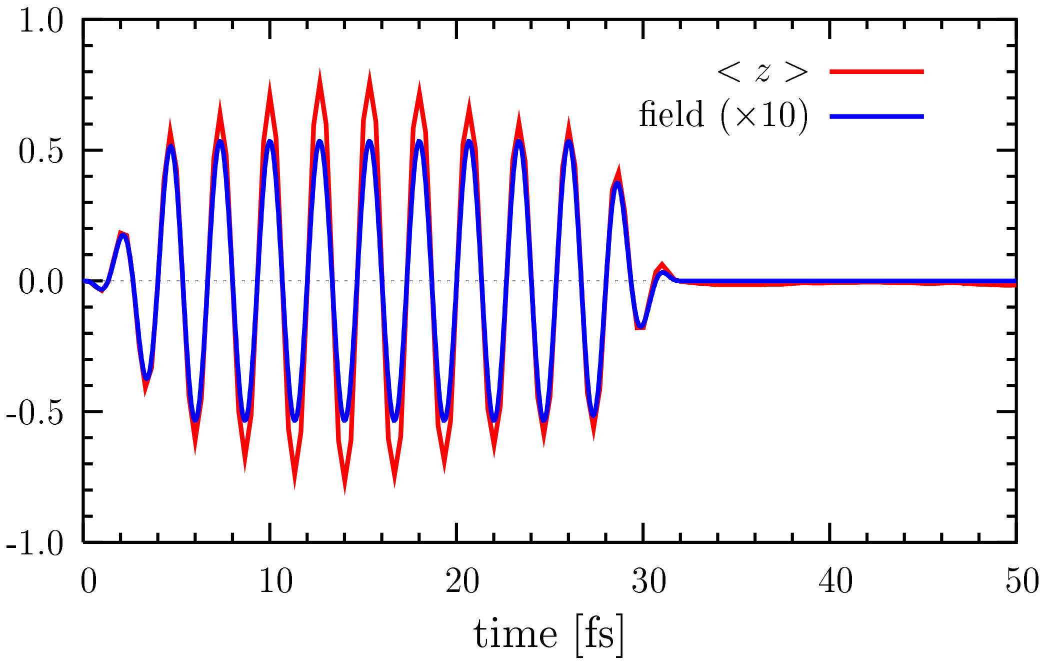
- Standard observables to calculate are $< R(t) >$ and $< z(t) >$.
- However, $< R(t) >$ has limited meaning since it includes vibration, dissociation, and Coulomb explosion; the same is true for $< z(t) >$.
- Looking at the complete nuclear and electronic distributions reveals significantly more information.
- In the following movies, watch for:
  - bond-stretching and bond-healing
  - vibrational excitation
  - dissociation (electron stays with one of the protons)
  - ionization (electron leaves the system, so protons undergo “Coulomb explosion”)
- Ultimately, we plan to project to particular final states to find, for example, the probability of exciting a particular vibrational and/or electronic state. In general, such a probability is given by

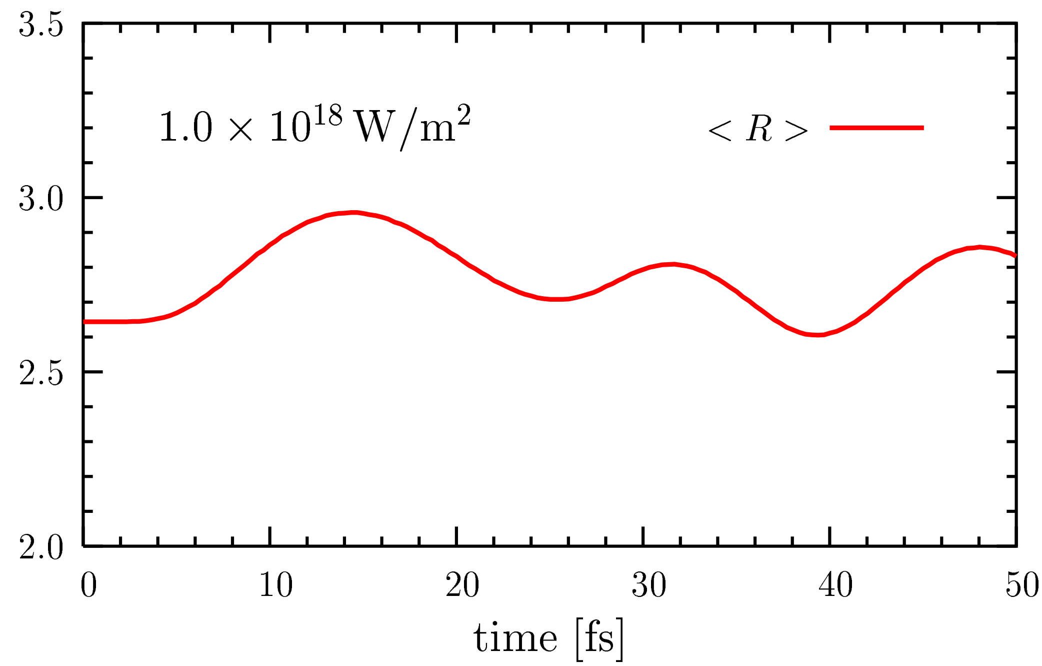
$$P_v^{n\sigma_{g,u}}(t) \equiv \left| \int_0^\infty dR \int_\infty^\infty dz \, F_v^{n\sigma_{g,u}}(R)\, G_R^{n\sigma_{g,u}}(z) \Psi(R, z, t) \right|^2$$

- To get a cross section, we need to take $\lim_{t\to\infty} P_v^{n\sigma_{g,u}}(t)$ and introduce a conversion factor.
- Similarly, we plan to determine ionization as well as dissociation cross sections.

Expectation Values

turn-on/off: 2 periods; on-time: 8 periods; time after: 8 periods





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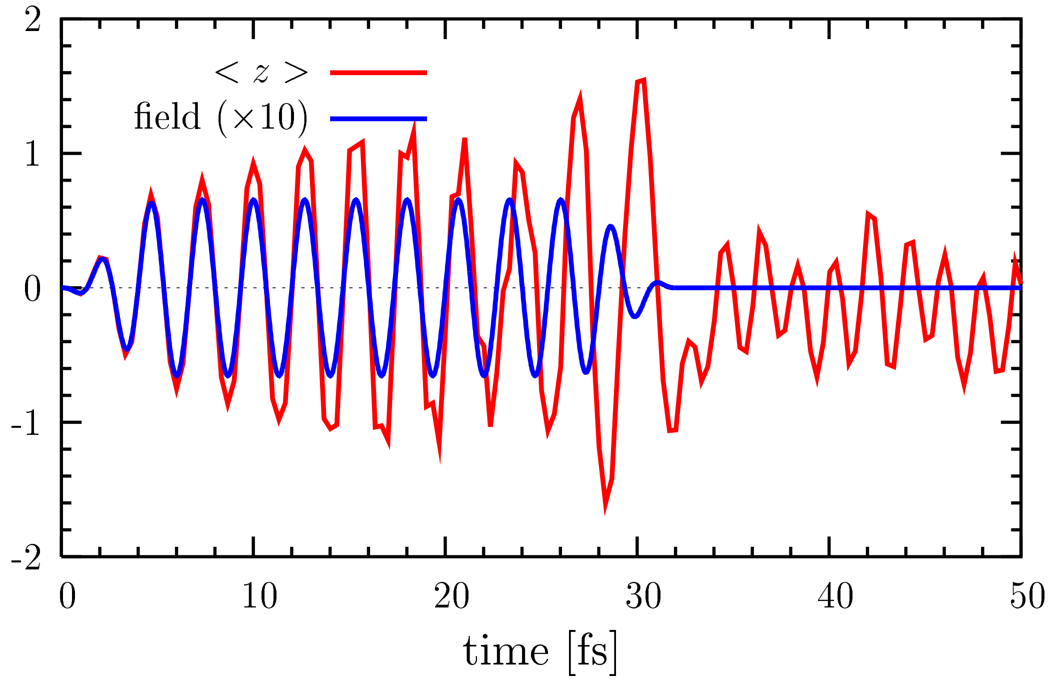

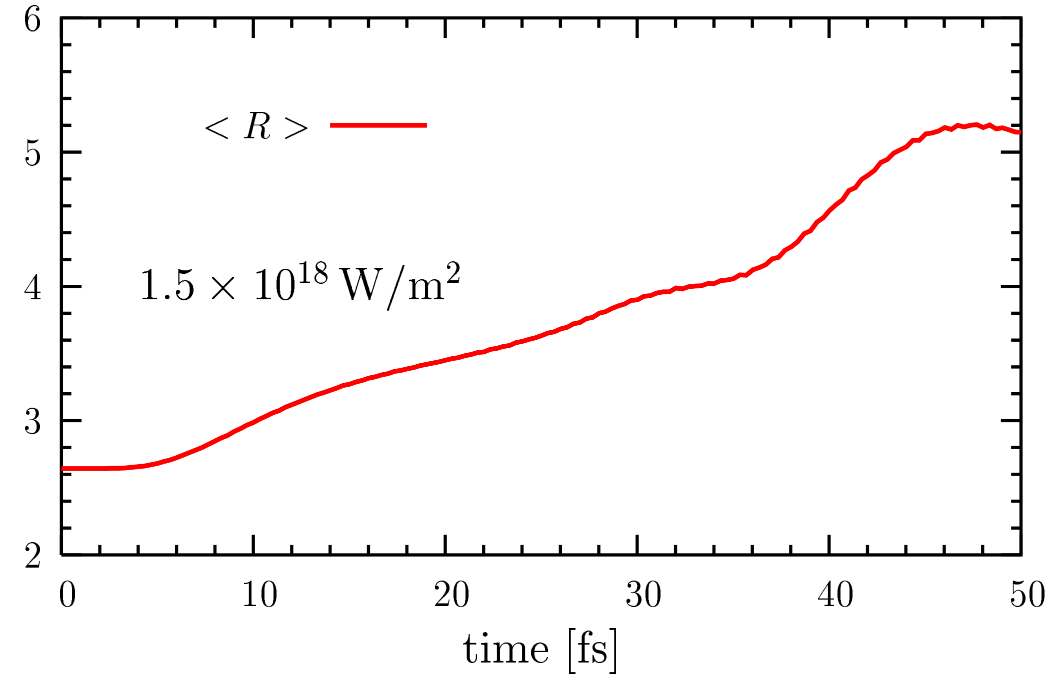

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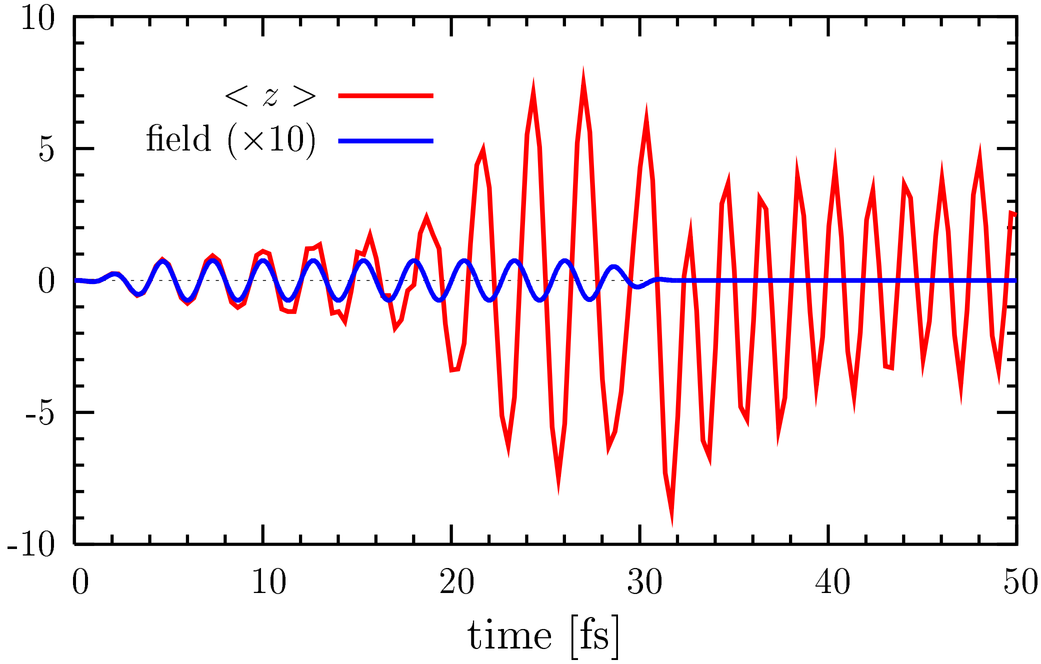
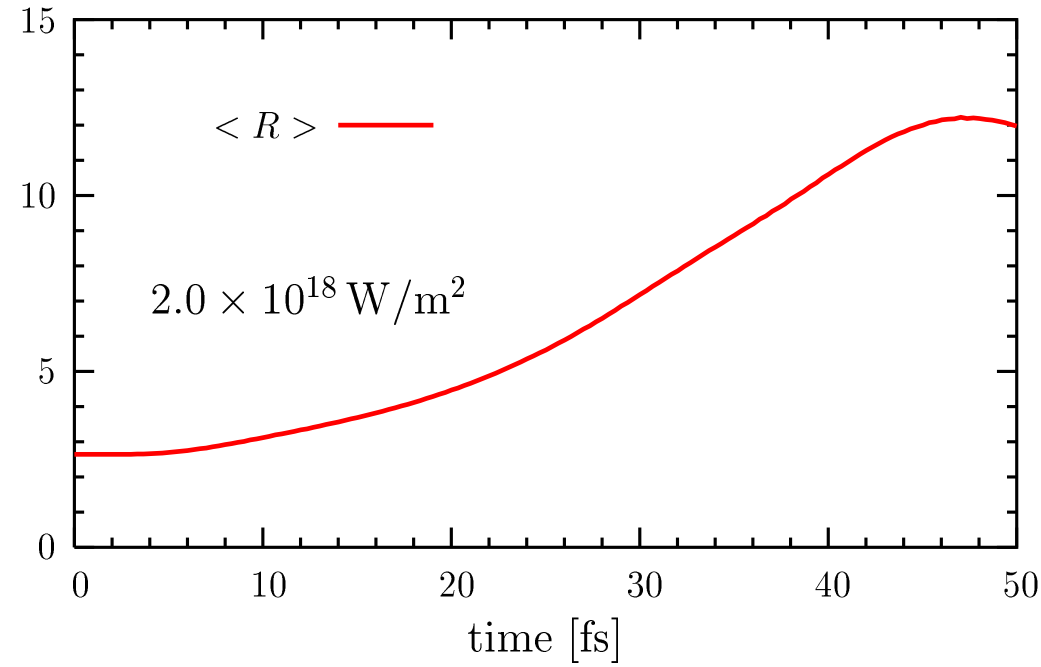
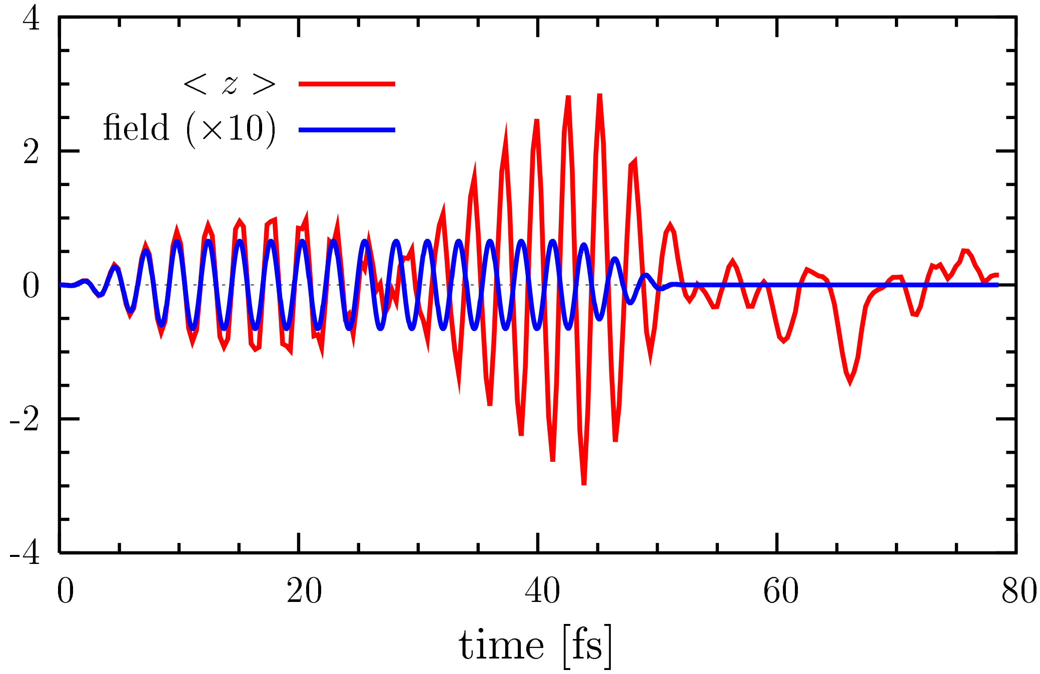
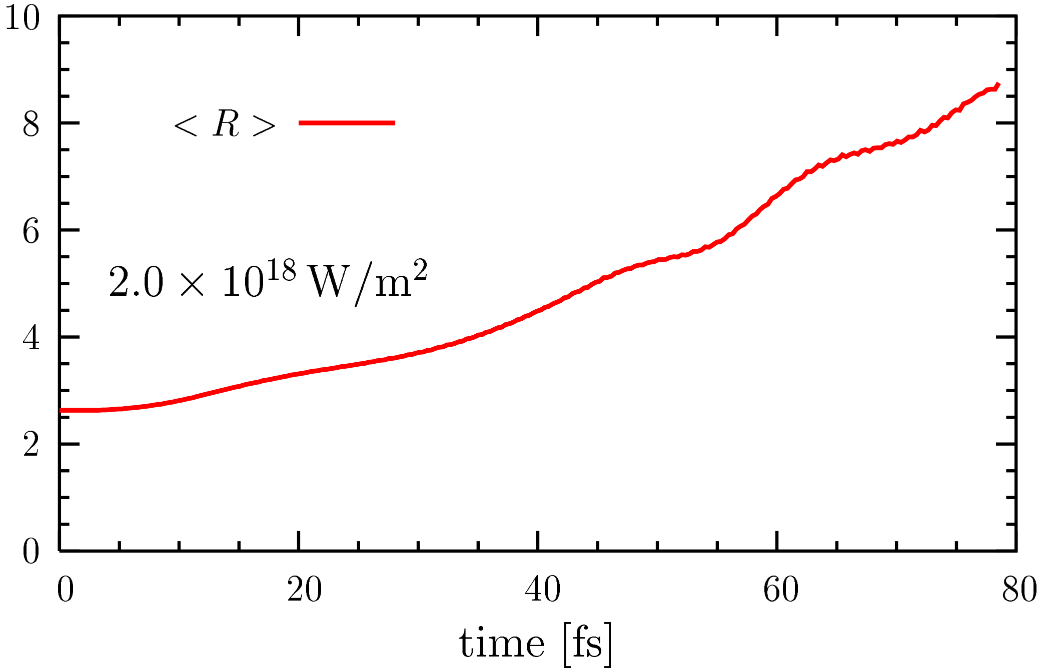




Expectation Values

turn-on/off: 4 periods; on-time: 12 periods; time after: 10 periods





Conclusions and Outlook

- Our method has been checked with good agreement against benchmark results for the Temkin-Poet model of e–H collisions [Phys. Rev. A 65 (2002) 060701(R)] and the H_2^+ 1D-problem.
- By avoiding boundary masking, we can extract useful physics about the final state of the system using simple projection methods.
- By projecting onto different states, we can separately find probabilities for excitation, ionization, and dissociation processes.
- We note the importance of watching the evolution of the system after the laser pulse is over (→ "bond healing").
- The Temkin-Poet code has been parallelized. We are in the process of doing the same for the H_2^+ problem, which will allow us to use even bigger grids and longer propagation times.
- Possibilities to extend the analysis beyond one dimension with two degrees of freedom will be explored.
- Movies have been created to enhance the visualization.