Parallelizable Algorithms for Describing the Effects of Strong Time-Dependent Electromagnetic Fields on the Hydrogen Atom

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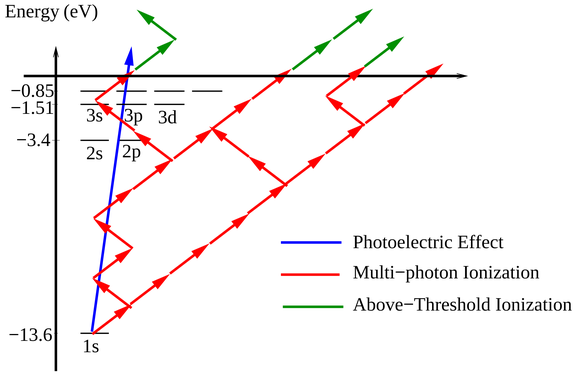
Abstract

We are testing a variety of methods to numerically treat the ionization of atomic hydrogen by a strong laser pulse. Besides providing high accuracy, the algorithms should be parallelizable in order to handle the sometimes long propagation times needed to solve the time-dependent Schrödinger equation for this fundamental strong-field problem. We report progress on developing a computer code that will make such calculations possible on massively parallel supercomputer platforms.

Introduction and Motivation

- **1 attosecond** is one-millionth of one millionth of one millionth (10^{-18}) of a second.
- There are twice as many attoseconds in 1 second than seconds in the **age of the universe** (15 billion years)!
- The period for the $n = 1$ orbit in atomic hydrogen is about 150 attoseconds.
- Attosecond laser pulses provide a window to study the details of (valence) electron interactions in atoms and molecules.
- A major role for **theory** in attosecond science is to **suggest novel ways of investigating and controlling electronic processes** in matter on ultra-short time scales.
- Typical laser intensities in this field range from 10^{12} to 10^{15} W/cm^2.
- **10^{14} W/cm^2 is a million billion times stronger than the radiation that the Earth receives from the Sun directly above us on a clear day.**
- Such intensities can rip electrons away from atoms in very different ways from the **standard photoeffect**:
  - **Multi-photon ionization**
  - **Above-threshold ionization**
  - **Field (tunnel) ionization**

Single vs. Multi−Photon Ionization in Atomic Hydrogen



The Problem

- We start with the **Time-Dependent Schrödinger Equation**

$$\hat{\boldsymbol{H}}\Psi = i\frac{\partial}{\partial t}\Psi \tag{1}$$

- In the **Length Form** of the electric dipole operator,

$$\hat{\boldsymbol{H}} = -\frac{1}{2}\boldsymbol{\nabla}^2 - \frac{1}{r} + r\cos(\vartheta)E(t) \tag{2}$$

- In the **Velocity Form**, we have instead

$$\hat{\boldsymbol{H}} = -\frac{1}{2}\boldsymbol{\nabla}^2 - \frac{1}{r} + i\frac{\boldsymbol{A}(t)}{c}\cdot\boldsymbol{\nabla} \tag{3}$$

- We currently propagate the initial wavefunction $\Psi(\boldsymbol{r}, t = 0)$ in time using **Finite Differences**.
- An alternative is to use **Finite Elements** (B-splines, discrete-variable representations).

Numerical Methods

Crank-Nicolson Approximation (CN)

$$\Psi(\boldsymbol{r}, t + \Delta t) \approx \frac{1 - i\hat{\boldsymbol{H}}\Delta t/2}{1 + i\hat{\boldsymbol{H}}\Delta t/2}\Psi(\boldsymbol{r}, t) \tag{4}$$

- This is an **implicit** method that allows for large timesteps.
- It is difficult to calculate the "denominator", i.e., the inverse of a matrix at every time step.
- Using typical finite differences for the second derivative, a tri-diagonal systems needs to be solved.
- Standard algorithms do not parallelize well — we are currently testing **PETSC**.

Matrix Iteration Method (MI)

- We define

$$1 + i\hat{\boldsymbol{H}}\Delta t/2 \equiv \hat{\boldsymbol{O}}_{\boldsymbol{D}} + \hat{\boldsymbol{O}}_{\boldsymbol{ND}} \tag{5}$$

- Then we expand

$$(1 + i\hat{\boldsymbol{H}}\Delta t/2)^{-1} \approx (\mathbf{1} - \hat{\boldsymbol{O}}_{\boldsymbol{D}}^{-1}\hat{\boldsymbol{O}}_{\boldsymbol{ND}} + \hat{\boldsymbol{O}}_{\boldsymbol{D}}^{-1}\hat{\boldsymbol{O}}_{\boldsymbol{ND}}\hat{\boldsymbol{O}}_{\boldsymbol{D}}^{-1}\hat{\boldsymbol{O}}_{\boldsymbol{ND}} + \ldots)\hat{\boldsymbol{O}}_{\boldsymbol{D}}^{-1} \tag{6}$$

- The inverse of the diagonal matrix $\hat{\boldsymbol{O}}_{\boldsymbol{D}}^{-1}$ is trivial.
- Taking 3−8 terms in the series expansion generally yields converged results.
- Calculating these terms by iteration again requires the solution of a tridiagonal system.

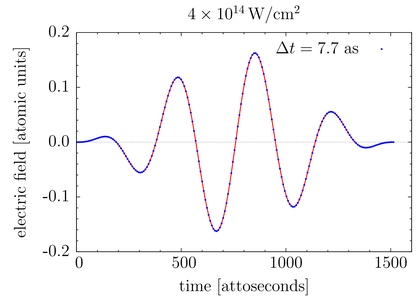
Leapfrog Approach (LF)

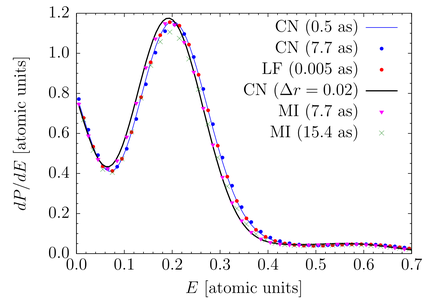
$$\Psi(t + \Delta t) = \Psi(t - \Delta t) - 2i\Delta t\hat{\boldsymbol{H}}\Psi(t) \tag{7}$$

- This is an **explicit** method that only allows for small timesteps.
- **Δt is limited by the radial stepsize Δr; $\Delta t \ll (\Delta r)^2$.**
- However, since only matrix-vector multiplications are involved
  - each step is very fast;
  - the method is ideal for parallelization.

Our Test Case

Ejected-electron energy distribution from a 4-cycle pulse with peak intensity 4×10^{14} W/cm^2 and central photon energy of 0.4 a.u.





Results and Discussion

method	Δr [a.u.]	$\Delta t_{\max}$ [10^{-18} s]	time steps	t_{step}[s]	t_{total} [s]
Crank-Nicholson (L)	0.06	7.7	195	0.048	9.33
Matrix Iteration (V)	0.06	7.7	195	0.197	38.39
Leapfrog (L)	0.06	0.0048	314158	0.014	4386

- We had to **choose a radial step of $\Delta r = 0.06$ a.u. to give LF any chance at all!**
- LF is accurate, each timestep is fast, but the individual steps are too small. **Even parallelization is unlikely to be worthwhile.**
- To use explicit methods, we need a bigger radial step without losing accuracy. **A possible way forward is a finite-element discrete-variable representation (FE-DVR).**
- **The accuracy of the implicit methods remains high for large timesteps** – a slight breakdown occurs at about 25 points per laser cycle.
- **The MI method is slower than CN**, but – for our example – can handle a larger step Δr.
- For strong infrared fields, **MI in the velocity form will probably win**, since it converges with far less coupled channels.
- It seems **highly worthwhile to speed up the solution of the tridiagonal system** – for example, by trying **PETSC**.