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

John Emmons, Austin Howes, Alex Kramer, X. Guan, K. Bartschat, J. Grout, and A. N. Grum-Grzhimailo

Department of Physics and Astronomy, Drake University, Des Moines, IA 50311, USA
Department of Mathematics and Computer Science, Drake University, Des Moines, IA 50311, USA
Institute of Nuclear Physics, Moscow State University, Moscow 119991, Russia
Research Supported by the United States National Science Foundation under PHY-1068140

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 (10^{-18}) of a second. 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^{13} to 10^{15} W/cm^2.

• 10^{15} 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

Energy (eV)

-0.85
-1.51
-3.44
-13.6

• We start with the Time-Dependent Schrödinger Equation

\[ \dot{\Psi} = -\frac{\partial}{\partial t} \Psi \]

• In the Length Form of the electric dipole operator,

\[ \dot{\Psi} = -\frac{1}{2} \nabla^2 \Psi + \frac{1}{2} \cos(\theta) \nabla \theta \]

• In the Velocity Form, we have instead

\[ \dot{\Psi} = -\frac{1}{2} \nabla^2 \Psi - \frac{1}{4} \cos(\theta) \nabla \theta \]

• We currently propagate the initial wavefunction \( \Psi(\mathbf{r}, t = 0) \) in time using Finite Differences.

• An alternative is to use Finite Elements (B-splines, discrete-variable representations).

Numerical Methods

Crank-Nicolson Approximation (CN)

\[ \frac{\Phi(\mathbf{r}, t + \Delta t) - \Phi(\mathbf{r}, t)}{\Delta t} \approx \frac{1}{2} \dot{\Phi}(\mathbf{r}, t) \]

• This is an implicit method that allows for large timesteps.

• It can be difficult to calculate the "denominator", i.e., the inverse of a matrix at every time step.

• Standard algorithms do not parallelize well — we are currently testing PETSC.

Matrix Iteration Method (MI)

\[ \Phi(\mathbf{r}, t + \Delta t/2) \approx O_{\Delta t/2} \Phi(\mathbf{r}, t) \]

• We define

\[ \Delta t = 0 \to 0.048 \text{ a.u.} \]

• Then we expand

\[ (1 + \dot{H} \Delta t/2)^{-1} \approx (1 - \hat{O}_{\Delta t/2} \hat{O}_{\Delta t/2})^{-1} \]

• The inverse of the diagonal matrix \( \hat{O}_{\Delta t/2} \) 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)

\[ \Phi(\mathbf{r}, t + \Delta t) = \Phi(\mathbf{r}, t) - 2\Delta t \hat{H} \Phi(\mathbf{r}, t) \]

• This is an explicit method that only allows for small timesteps.

• \( \Delta t \) is limited by the radial stepsize \( \Delta r \); \( \Delta t \ll (\Delta r)^2 \).

• However, since only matrix-vector multiplications are involved — each step is very fast.

• The method is ideal for parallelization.

Results and Discussion

Electron-electron energy distribution from a 4-cycle pulse with peak intensity \( 4 \times 10^{14} \text{ W/cm}^2 \) and central photon energy of 0.4 a.u.

- We had to choose a radial step of \( \Delta r = 0.06 \text{ a.u.} \) 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 help worthwhiler.

- 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 \( \Delta r \).

- 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.