PyProp - A Python Framework for Propagating the Time Dependent Schrödinger Equation

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Underlying Goal

Study the behaviour of atoms and molecules

Length Scale

10^0m	Humans
10^{-2}m	Golf balls
10^{-4}m	Width of human hair
10^{-6}m	Cells
10^{-8}m	Vira
10^{-10}m	Atoms

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How?

- Atoms are smaller than the wavelength of light
- Any observation leads to a modification of the system
- It is not possible to directly observe what is going on
- Need theoretical models and calculations to match experiments

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Numerical Experiment

Simulation of an experimental setup on a computer

1. An atomic/molecular system is in an initial state
2. The system interacts with an external force
   - Interaction with radiation (laser)
   - Collision with another atom/ion/molecule
3. The final state of the system is analyzed to compare with experiments

The goal of this thesis is to perform steps 1 and 2 and simplify step 3 for a wide range of problems

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Outline

- Overview of the thesis
- Introduction to Quantum Mechanics
- Solving the Time Dependent Schrödinger Equation on a computer
- How PyProp is a flexible solver
- Applying PyProp to laser ionization of Helium

Thesis Overview

Development and application of PyProp

- Computer Science - Software design and implementation
- Mathematics - Numerical methods
- Physics - Applications

What is PyProp?

Framework for solving the Time Dependent Schrödinger Equation

- Goals
  - Flexibility
  - Performance
- Research tool, not QM@Home
  - Common tasks automated
  - Difficult tasks possible
- Free Software (GPL) http://pyprop.googlecode.com

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Classical Mechanics

A classical particle has a well defined position and velocity.

The change of velocity is described by Newton's Law

$$\mathbf{F} = m\mathbf{a}$$

Quantum Mechanics

Heisenberg uncertainty principle: a particle can not have well defined position and velocity

- There is a probability for finding a particle in a given position
- Must therefore consider all possible positions at the same time

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Mathematical Formulation

Position and velocity is replaced by a *wavefunction*

$$\psi(\mathbf{x}, t)$$

$|\psi(\mathbf{x}, t)|^2$ is the probability density of finding the particle in $\mathbf{x}$

Time evolution of $\psi(\mathbf{x}, t)$ is described by the Time Dependent Schrödinger Equation (TDSE).

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x}, t) = \widehat{H}\psi(\mathbf{x}, t)$$

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Hamiltonian

The Hamiltonian describes the energies in the system

$$\widehat{H} = -\frac{1}{2m}\nabla^2 + V(\mathbf{x}, t)$$

- The differentiation operator represents kinetic energy
- $V(\mathbf{x})$ is the potential energy.
- Systems are characterized by different potentials

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Adding Particles

- Adding a particle is equivalent to adding degrees of freedom

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x}_1,\mathbf{x}_2,t) = \left(H_1(\mathbf{x}_1) + H_2(\mathbf{x}_2) + H_{1,2}(\mathbf{x}_1,\mathbf{x}_2)\right)\psi(\mathbf{x}_1,\mathbf{x}_2,t)$$

- The time for solving a system increases exponentially with the number of particles
  - 1 particle: 1 sec
  - 2 particles: 17 min
  - 3 particles: 277 hours
  - 7 particles: age of the universe
- The "exponential wall" of quantum mechanics

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Computational Quantum Mechanics

Returning to the TDSE

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \widehat{H}\psi(\mathbf{x},t)$$

Problem: if we know the $\psi(\mathbf{x},t)$, find $\psi(\mathbf{x},t+h)$.

- Can only be solved by hand for the simplest systems
- Computers does not work on continuous problems, the TDSE must therefore be *discretized* in space and time.

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Choice of coordinate system

Must choose a coordinate system in which to represent the multi-dimensional wavefunction.

- Cartesian coordinates, $\mathbf{x} = (x, y, z)$
- Spherical coordinates, $\mathbf{x} = (r, \theta, \phi)$
- Cylindrical coordinates, $\mathbf{x} = (r, \rho, \phi)$
- Each rank may be discretized independently
- Optimal choice is system dependent

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Discretization

- Approximating the continuous problem with a finite number of states.
- Sum of continuous basis functions

$$\psi(x,t) \approx \sum_{i=0}^{m} c_i(t) B_i(x)$$

- Perform calculations on $\mathbf{c}(t) = \{c_i(t)\}$
- Which basis functions should we use?
  - Fourier functions?
  - Orthogonal polynomials?
  - B-Splines?
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  - B-Splines?
- Optimal choice is system dependent

Propagation

Given a discretization scheme, we can turn the TDSE from

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \widehat{H}\psi(\mathbf{x},t) \qquad \rightarrow \qquad \mathrm{i}\mathbf{S}\frac{\partial}{\partial t}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t)$$

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- System dependent choices
  - coordinate system
  - discretization scheme
  - propagator
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- Independent Modules
- User Code

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Core	Wavefunction	Distribution
	Representation	Python Interface

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Discretization
- Equidistant Grid
- B-Splines
- Spherical Harmonics
- Orthogonal Poly.

Propagation
- Split-Step
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- IRAM Solver

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Flexibility

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  - Using high performance libraries where possible
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Current Applications

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Example: Laser Ionization of Helium

- Two electron system

$$\widehat{H}_0(\mathbf{r}_i) = -\frac{1}{2}\nabla^2 - \frac{2}{r_i} + A_z(t)\left(\frac{\partial}{\partial z_i} - \frac{\cos\theta_i}{r_i}\right)$$

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Helium in PyProp

- Three computational ranks
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- Total wavefunction has $\approx 10\,\mathrm{M}$ elements
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- Propagation with the Cayley Propagator
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  - Energy distribution
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Helium - Movie

Animation of an ionization event

Helium - Ionzation Probability

Ionization probability as a function of field strength

- Ionization probability does not go to one
- Each point on the graph is from one ionization event
  - Total of 30000 CPU hours

Summary

- Created a software framework for atomic physics
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Image Sources

Wikimedia Commons

- Vitruvian man - File:Vitruvian.jpg
- Hair - File:Human_Hair_40x.JPG
- Cell - File:SEM_blood_cells.jpg
- HIV - File:HIV-budding-Color.jpg
- Atom - File:Stylised_Lithium_Atom.svg

Raymond Nepstad

- Wavefunction
- Helium animation