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

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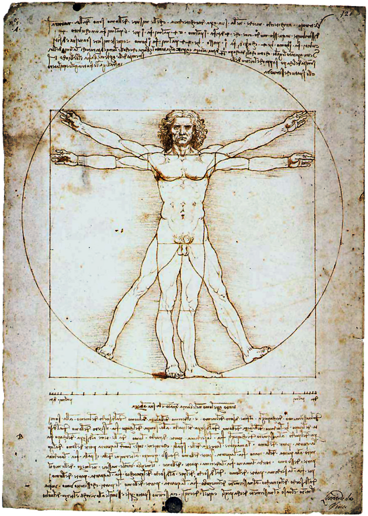
Study the behaviour of atoms and molecules



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| $10^{0}\mathrm{m}$ | Humans |
| $10^{-2}\mathrm{m}$ | Golf balls |
| $10^{-4}\mathrm{m}$ | Width of human hair |
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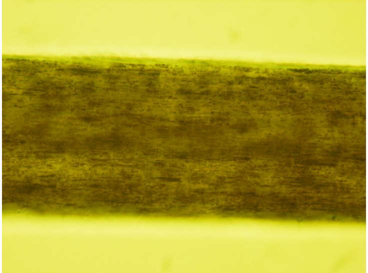

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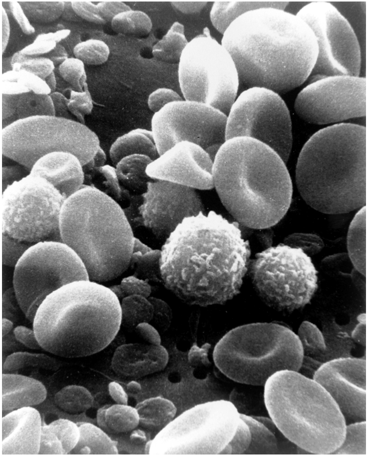

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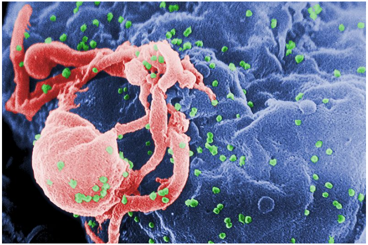

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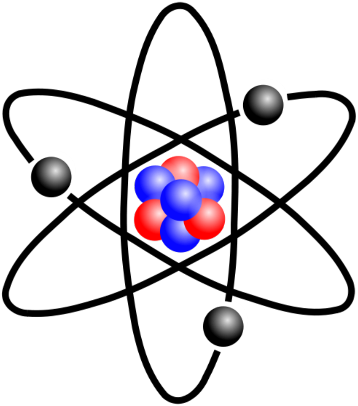

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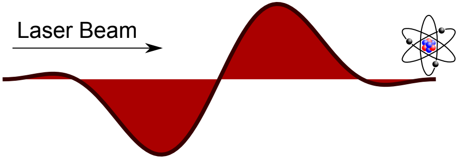
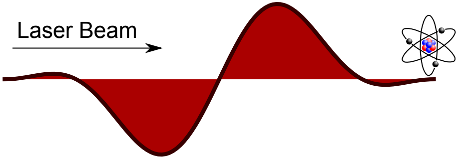



- Atoms are smaller than the wavelength of light
- Any observation leads to a modification of the system
- It is not possible to directly observe what is going on
- Need theoretical models and calculations to match experiments

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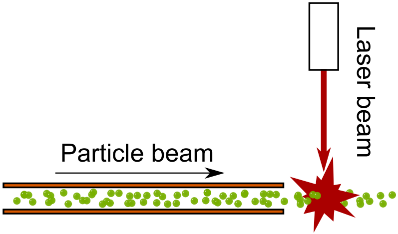


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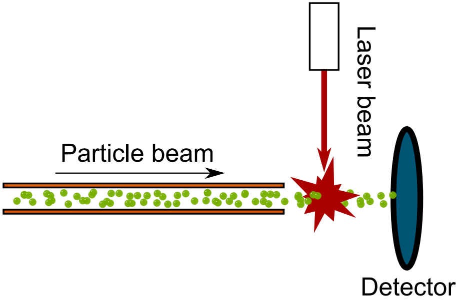


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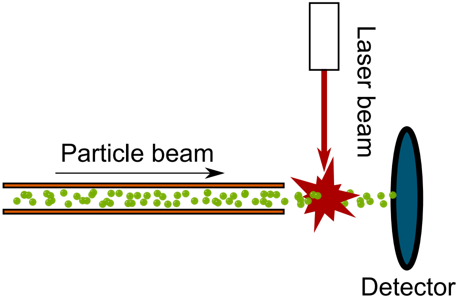


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*Simulation of an experimental setup on a computer*

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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- 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

Development and application of PyProp

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

*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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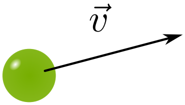
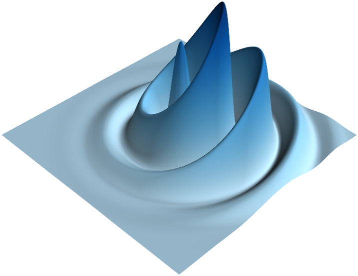



A classical particle has a well defined position and velocity.

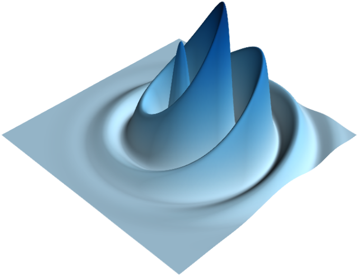
The change of velocity is described by Newton's Law

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



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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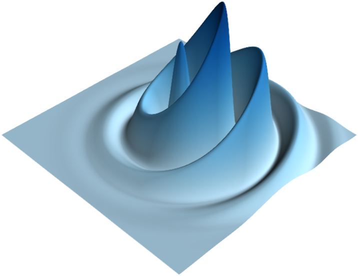

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Position and velocity is replaced by a *wavefunction*

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

$|\psi(\mathbf{x}, t)|^2$ 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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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 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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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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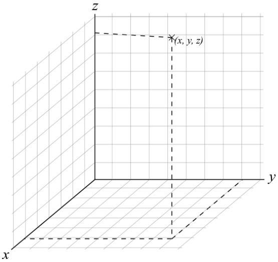
Problem: if we know the $\psi(\mathbf{x},t)$, find $\psi(\mathbf{x},t+h)$.

- 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.

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

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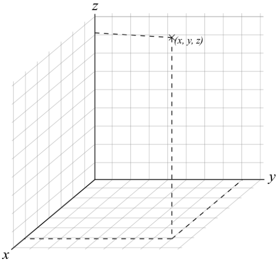


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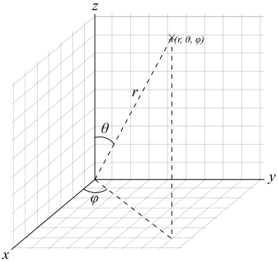


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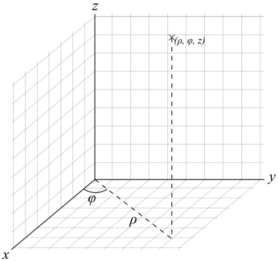


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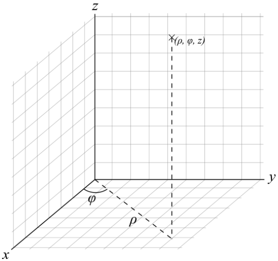


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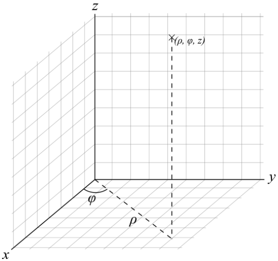


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- Approximating the continuous problem with a finite number of states.
- Sum of continuous basis functions

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

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|---|---|---|
| | Wavefunction | Distribution |
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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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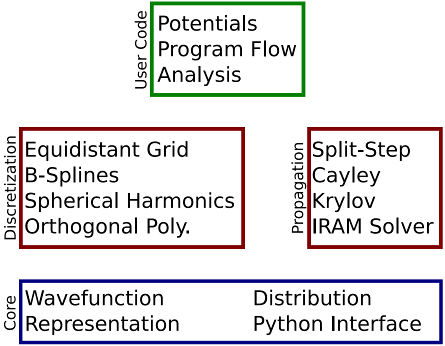

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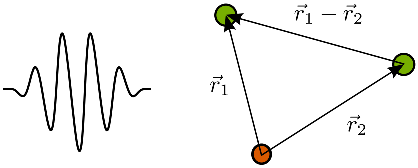


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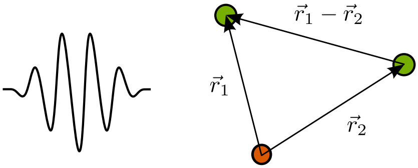


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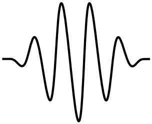

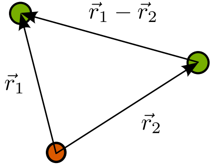


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  1. $\mathcal{Y}_{l_1,l_2}^{L,M}(\Omega_1,\Omega_2)$ - Combination of all angles
  2. $r_1$ - distance from nucleus to first electron
  3. $r_2$ - distance from nucleus to second electron
- Discretizing $r_1$ and $r_2$ with B-Splines
- Total wavefunction has $\approx 10\,\mathrm{M}$ elements
  - Total memory requirement is $\approx 100\,\mathrm{GB}$
  - Must be run in parallel
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  - Energy distribution
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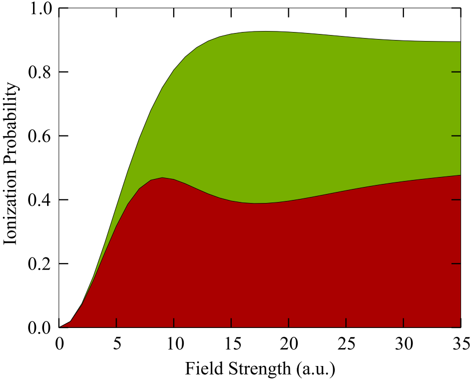
Animation of an ionization event

## 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

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- Atom - File:Stylised_Lithium_Atom.svg

**Raymond Nepstad**

- Wavefunction
- Helium animation