

Interactions of Intense, Ultra-Short Lasers with Atoms Fall 2010

Dan Walsh
Dept. Of Mathematics
UMass Dartmouth
Dartmouth MA 02747
Email: dwalsh1@umassd.edu

Abstract

We study interactions of intense, ultra-short laser pulses with atomic systems in the strong perturbation regime. Laser matter interactions are of current interest in research in atomic, molecular, and optical physics. In our project, numerical solutions of the time dependent Schrodinger equation of atomic systems interacting with a strong laser will be investigated. We will use a numerical method where the spatial coordinate is discretized on a grid and the temporal evolution is carried out using the Runge-Kutta scheme. We refer to this as the space-discretized Runge-Kutta (SDRK) method. The results of the SDRK method will be compared to those of other methods such as the split operator approach in terms of effectiveness and stability. The wavefunctions of model systems will be calculated and relevant properties such as ionization rates will be studied as a function of laser intensity and duration. We will also compare such exact numerical solutions with often used approximations such as the strong field approximation to study their validity.

Introduction

The Schrodinger Equation: A brief History

By the end of the 19th century, it was becoming quite clear that classical mechanics failed to explain all observed phenomena in the universe. With blackbody radiation disrupting our idea of a perfectly continuous physical world, and the wave particle duality matter discovered by de Broglie, it was time for a new formalism to explain the behavior of matter on the atomic scale. Using primarily the wave-particle duality of matter, Erwin Schrodinger set out to define a wavefunction, ψ , which is used to represent all possible positions a particle can occupy. [2]

Conditions of the Wavefunction: The Postulates

Erwin Schrodinger postulated the following regarding the wavefunction:

- Postulate 1: A particle may be described by a wavefunction, $\psi(\vec{r}, t)$, which is typically complex, but may be real. i.e. $\psi(\vec{r}, t) = R(\vec{r}, t) + iI(\vec{r}, t)$, where R is the real part, and I is the imaginary. A theorem in mathematics proves (rather tediously) that if $\psi(\vec{r}, t)$ is to describe a time dependent process, then $\psi(\vec{r}, t)$ is complex. We will make use of this fact when deriving our Time-dependent equation.
- Postulate 2: The probability of finding the particle described by the wave equation at time t in a volume dV, at position \vec{r} is given by

$$Pr(\vec{r}, t) = |\psi(\vec{r}, t)|^2 dx dy dz$$

Restraints on the Wavefunction

Our wavefunction must additionally obey the following:

- Continuity: Our wavefunction must be continuous everywhere
- Smoothness: The derivative of our wavefunction must also be continuous everywhere
- Unitarity: $\int_{-\infty}^{\infty} |\psi(\vec{r}, t)|^2 dr = 1$

A Heuristic Derivation of the Time Dependent Schrodinger Equation

From our earlier mentioned theorem, we must implement a complex wavefunction that is both space and time dependent. We assume it is of the simplest form: a plane wave, of the form

$$\psi(x, t) = Ae^{i(\frac{p}{\hbar}x - \frac{E}{\hbar}t)}$$

which describes a particle with momentum p and energy E. Taking a first order derivative with respect to x gives

$$\frac{\partial}{\partial x} \psi(x, t) = Ae^{i(\frac{p}{\hbar}x - \frac{E}{\hbar}t)} \frac{\partial}{\partial x} i(\frac{p}{\hbar}x - \frac{E}{\hbar}t) = Ae^{i(\frac{p}{\hbar}x - \frac{E}{\hbar}t)} * \frac{i p}{\hbar} = \frac{i p}{\hbar} \psi(x, t)$$

taking a second x derivative simply gives

$$\frac{\partial^2}{\partial x^2} \psi(x, t) = \frac{\partial}{\partial x} \frac{i p}{\hbar} \psi(x, t) = \frac{i p}{\hbar} \frac{\partial}{\partial x} \psi(x, t) = (\frac{i p}{\hbar})^2 \psi(x, t) = -(\frac{p}{\hbar})^2 \psi$$

or simply

$$p^2 \psi(x, t) = -\hbar \frac{\partial^2}{\partial x^2} \psi(x, t)$$

There is a very important feature in quantum mechanics to take note of here. Momentum is no longer simply a value, but instead an operator, along with its square. The same can be said of any arbitrary function of x , like a potential, $V(x)$, where

$$V(x)\psi(x, t) = V(x)\psi(x, t)$$

So there is no actual calculation required. From classical mechanics, we can express the net energy of the system (potential and kinetic) as the Hamiltonian,

$$E = H = T + V = \frac{p^2}{2m} + V(x)$$

Using our notion of operators, we can extend this to a quantum mechanical system:

$$E\psi(x, t) = \hat{H}\psi(x, t) = \frac{p^2}{2m}\psi(x, t) + V(x)\psi(x, t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x, t) + V(x)\psi(x, t)$$

To get E , we simply need to take a first time derivative of our planewave.

$$\frac{\partial}{\partial t}\psi(x, t) = -\frac{iE}{\hbar}\psi(x, t) = \frac{E}{i\hbar}\psi(x, t)$$

or

$$i\hbar\frac{\partial}{\partial t}\psi(x, t) = E\psi(x, t)$$

Substituting for E in our energy equation, we get

$$i\hbar\frac{\partial}{\partial t}\psi(x, t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x, t) + V(x)\psi(x, t)$$

which is the Time Dependent Schrodinger Equation in 1 Dimension [1]. If we wish to extend this to 3-D, we would have

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r}, t) = \frac{-\hbar^2}{2m}\nabla^2\psi(\vec{r}, t) + V(\vec{r})\psi(\vec{r}, t)$$

The Time Independent Schrodinger Equation

If we make our wavefunction a product of time and space dependent functions, we have

$$\psi(x, t) = U(x)T(t)$$

which allows us to arrive at the equations

$$\hat{H}U(x) = EU(x)$$

and

$$T(t) = Ae^{-i\frac{E}{\hbar}t}$$

where E is the eigenvalue of the Hamiltonian operator, and the associated energy of the particle.

Numerical Evaluation of the TDSE

We first start by working in the atomic unit system, where $m=\hbar = 1$, so our TDSE becomes

$$\iota \frac{\partial}{\partial t} \psi(x, t) = -\frac{1}{2} \frac{\partial^2}{\partial x^2} \psi(x, t)$$

we can approximate the spatial derivative on the right hand side by discretizing our space into n space steps, and considering the j th step

$$\frac{\partial^2}{\partial x^2} \psi(x, t) \sim \frac{\psi_{j-1}(t) - 2\psi_j(t) + \psi_{j+1}}{h^2}$$

where h is the step size, plugging this into the TDSE will result in an ODE with respect to time

$$\iota \frac{d}{dt} \psi_j = -\frac{1}{2} \frac{\psi_{j-1}(t) - 2\psi_j(t) + \psi_{j+1}}{h^2} + V_j \psi_j$$

Since our wavefunction is describing a time dependent process, we again use our theorem to state that our wave function must indeed be complex, then we may split it up into real and imaginary parts by $\psi_j = R_j + \iota I_j$. Substituting this value gives a system of coupled ordinary differential equations in t

$$\frac{d}{dt} R_j = -\frac{1}{2} \frac{I_{j-1} - 2I_j + I_{j+1}}{h^2} + V_j I_j$$

and

$$\frac{d}{dt} I_j = \frac{1}{2} \frac{R_{j-1} - 2R_j + R_{j+1}}{h^2} - V_j R_j$$

The Leapfrog Method: A classical example

One area of interest of this project, before attempting to undertake any numerical evaluations of the coupled system, was to investigate the effectiveness of the Leapfrog integration scheme versus forward Euler integration. In order to do so, a classical example was used, given the initial position, velocity, and potential, one could use the leapfrog method through the following three equations.

$$x_{1/2} = x_0 + v_0 * \frac{h}{2}$$

$$v_1 = v_0 + a(x_{1/2}) * \frac{h}{2}$$

$$x_1 = x_{1/2} + v_1 * \frac{h}{2}$$

Here it becomes obvious where it gets its name from. It evaluates x at the halfway mark, then leaps over to evaluate v at the next step, then leaps over again to get x at the next integer step, and so on..

One particular thing of importance regarding the leapfrog integration scheme is that it preserves area in phase space, something that forward Euler does not do. What typically ends up happening as a result of phase space area not being preserved is that the system will end up gaining energy, which violates conservation laws, as we will see later.

Propagation of Time Independent solutions and The Principle of Superposition

As we saw earlier, our wavefunction could be broken up into temporal and spatial components, and their product would yield the solution. Since our spatial wavefunction gives us an eigenvalue problem, our solutions to this problem, $U(x)$, will form an orthonormal basis in a Hilbert space, which is typically infinite dimensional, with a few exceptions. The principle of superposition states that any state ψ is the sum of all possible eigenstates, with proper normalization coefficients. Or rather

$$|\psi\rangle = \sum_{n=1}^{\infty} c_n |n\rangle$$

where $|\psi\rangle$ is the state vector, and $|n\rangle$ is the n th eigenstate, and c_n^2 is the probability of our wavefunction being found in that state. If we wish to get the time evolution of our system, we simply multiply it upon our temporal function to get

$$|\psi(t)\rangle = \sum_{n=1}^{\infty} c_n |n\rangle e^{-\frac{iE_n}{\hbar}t}$$

Where E_n is the eigenvalue corresponding to the n th eigenstate.

1 Leapfrog Method in a Harmonic Potential

To test the effectiveness of the leapfrog method, it was implemented on a well known potential: the harmonic oscillator. Euler's Method was also used to compare the solutions, which can be viewed in the following figures. Noticeably, the amplitude in the Euler solution seems to be increasing with time, which is a result of the inaccuracy of a first order method like Forward Euler. We can see additional problems in Euler that

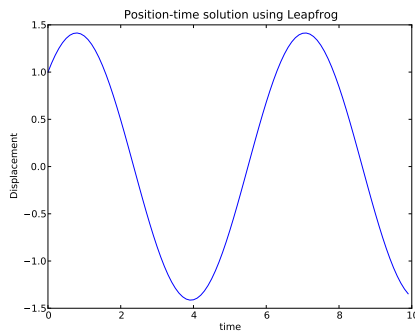


Figure 1: Leapfrog Method Solution

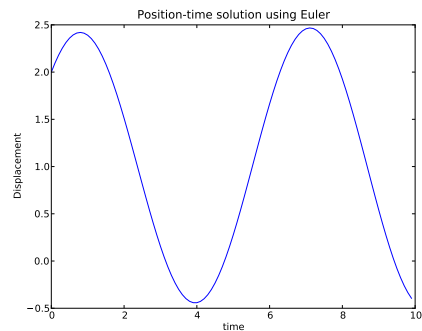


Figure 2: Eulers Method Solution

we don't see in higher order schemes like leapfrog in their respective energy plots in figures 3 and 4. It is apparent that the energy seems to be increasing linearly with time for the Euler scheme, while remaining constant as it should with leapfrog.

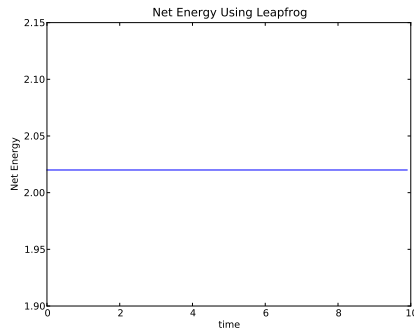


Figure 3: Leapfrog Method Energy

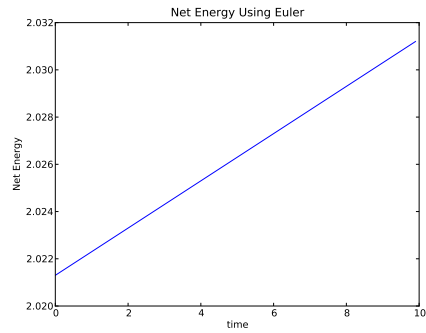


Figure 4: Eulers Method Energy

Qualitative analysis of the time evolution of a particle in a box

Using the principle of superposition, the time evolution of a particle in a box was qualitatively analyzed using VPython as the tool for analysis. For a particle in a box of length L , the n th eigenstate is given by

$$|n\rangle = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

with eigenenergy $E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2}$. Plotting the norm squared gave the probability density function for our particle. The probability density started off as a single peak, then expanded, eventually splitting into 2 peaks of equal height, and then returning to its original peak, suggesting that the probability of finding a particle at some point in the box was periodic in time.

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References

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