X-rays Emission from Atoms Driven by Ultrafast Lasers

Mendilyi Yohanna*, Anatole Kenfack

African Institute for Mathematical Sciences (AIMS) – Senegal*
Free University Berlin - Germany

AIMS SÉNÉGAL
African Institute for Mathematical Sciences

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THE GOAL

We want to generate coherent beams at shorter wavelengths, within the spectrum region of X-Rays or Extreme Ultraviolet (XUV) [2] from a femtosecond laser light. To proceed, we use a technique known as High Harmonic Generation (HHG) in which the mechanism behind it is a three-step model.

THE MODEL

Our model consists of a single Hydrogen atom (H) driven by a strong laser field E(t). The one dimensional Hamiltonian of such a system in atomic units ($\hbar$ = m = e = 1) reads:

$$H(x,t) = \frac{P^2}{2} + V(x) - xE(t)$$

where x and P are the position and the momentum of the particle, respectively, and $V(x) = -1/\sqrt{x^2+a^2}$ is the soft-core potential with the softening parameter a. Here E(t) stands for the linear polarized laser field which we have chosen as follows: E(t) = E_0 cos(ωt), where E_0 is the laser amplitude and ω its frequency. The system can be described by the following Time Dependent Schrödinger Equation (TDSE):

$$i\frac{\partial \Psi(x,t)}{\partial t} = H(x,t)\Psi(x,t)$$

where Ψ(x,t) is the time dependent wave packet or wave function. It turns out that the solution Ψ(x,t) can be formally written as:

$$\Psi(x,t) = U(t,t_0)\Psi(x,t_0)$$

where $U(t,t_0) = \exp(-iH(x,t)(t-t_0))$ is the unitary operator obtained, assuming that $t - t_0 = \Delta t$ is infinitesimally small, $\Psi(x,t_0)$ is the initial wave function which in general is the ground state wave function of the system.

SOLVING THE TDSE

To proceed, we used the FFT (Fast Fourier Transform) Split Operator method. Briefly speaking, this consists of splitting the above unitary operator as follows:

$$\Psi(x,t) = exp(-iV(x,t)\Delta t/2)exp(-iT\Delta t)exp(-iV(x,t)\Delta t/2)\Psi(x,t_0)$$

where V(x,t) = V(x) − xE(t) is the time dependent potential and $T = P^2/2$ the kinetic energy. The solution Ψ(x,t) is thus obtained executing the following algorithm:

i) Multiply exp(−iV(x,t) Δt/2) with $\Psi(x,t_0)$,
ii) Fast Fourier Transform the result of i) ,
iii) Multiply exp(−iT Δt) with result of ii),
iv) Inverse Fast Fourier Transform the result of iii),
v) Multiply exp(−iV(x,t) Δt/2) by the result of iv).

The above algorithm has been implemented using the Scilab programming language. The initial wave packet has been arbitrarily taken as:

$$\Psi(x,t_0) = exp(-\alpha x^2)$$

Note that well desired spectra will be obtained with suitable laser femtosecond laser pulse and starting the propagation from the true ground state of the H atom. This ground state can be obtained by the so-called imaginary time propagation.

THE HIGH HARMONIC GENERATION (HHG)

>>Three-Step Model (TSM)

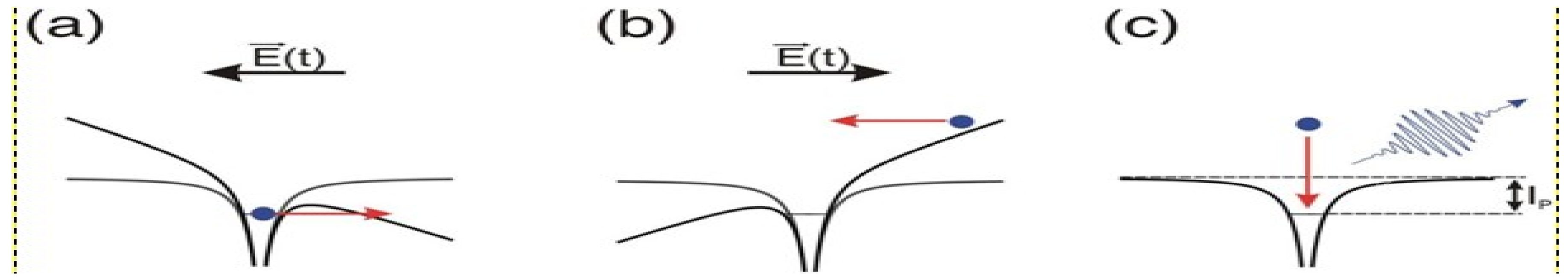

Figure 1: Three step model. (a) Tunneling, (b) Acceleration, (c) Recombination.

(a) The electron is bound by the Coulomb potential of an atom. An incoming intense laser field distorts the potential and allows the tunneling of the electron through the Coulomb barrier.
(b) The free electron is accelerated away from its parent ion by the laser field. After half an optical cycle, the sign of the laser field reverses, this leads to an acceleration back towards the ion.
(c) The electron recombines with its parent ion and emits a photon with a photon energy composed of the, Ionization energy of the atom I_p and the kinetic energy of the electron gained by its interaction with the laser field.

THE EMISSION SPECTRA

The emission spectra is given by:

$$\sigma(\omega) = |\int_0^\infty \langle \ddot{x} \rangle(t) \exp(-i\omega t)dt|^2$$

Where $\langle \ddot{x} \rangle(t) = \langle \Psi(x,t) \mid -\partial V(x)/\partial x + E(t) \mid \Psi(x,t) \rangle$ stands for the dipole acceleration.

IMPLEMENTATION AND RESULTS

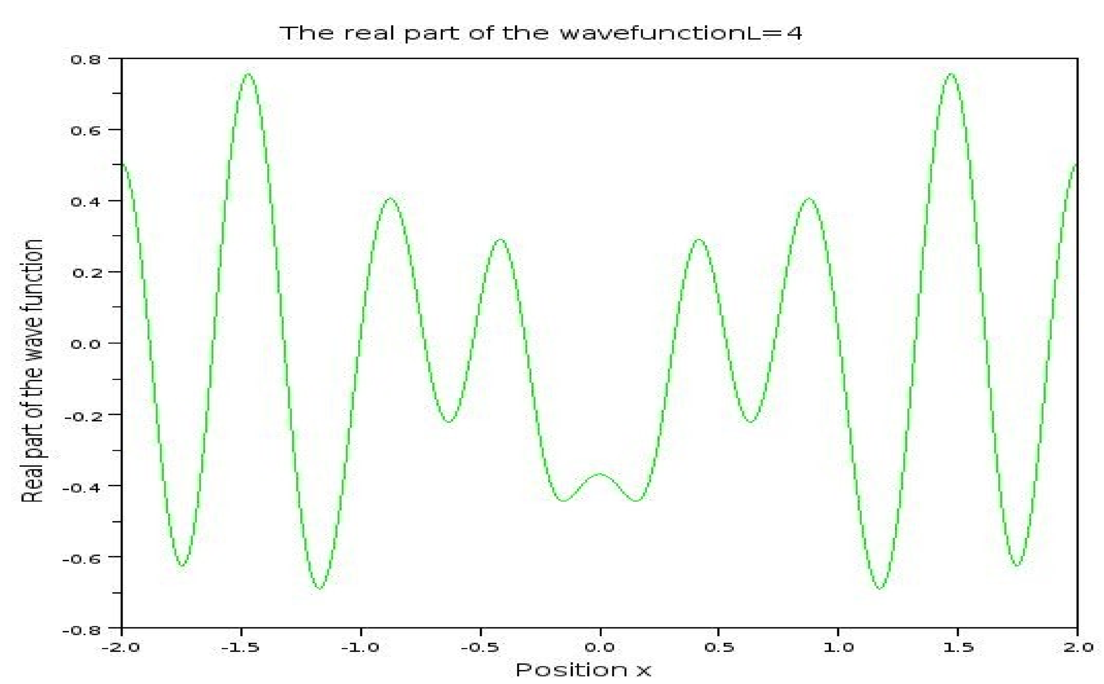

Figure 2: The real part of the wave function on the grid of spatial length L=4.

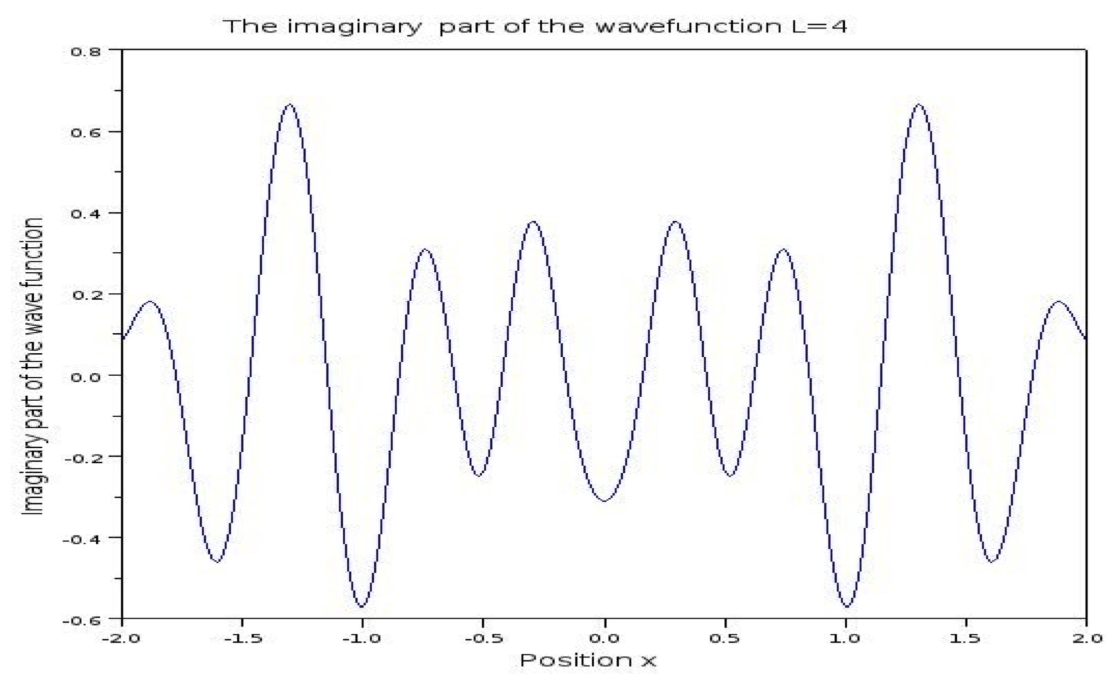

Figure 3: The imaginary part of the wave function as a function of x for spatial length L=4.

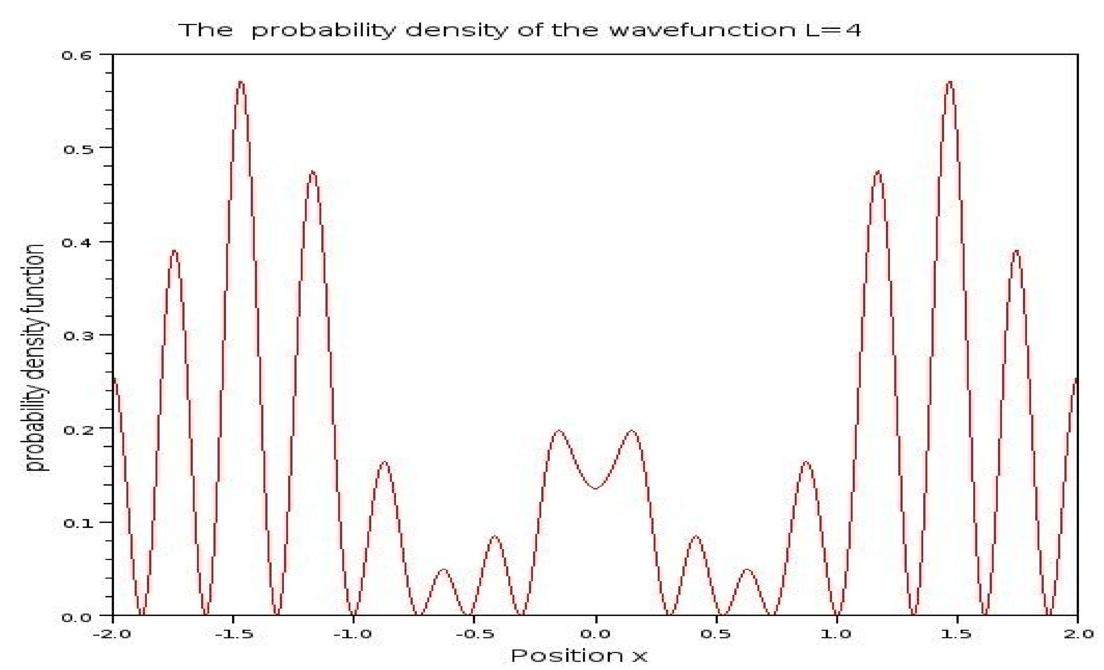

Figure 4: The probability density of the wave function as a function of x for spatial length L=4.

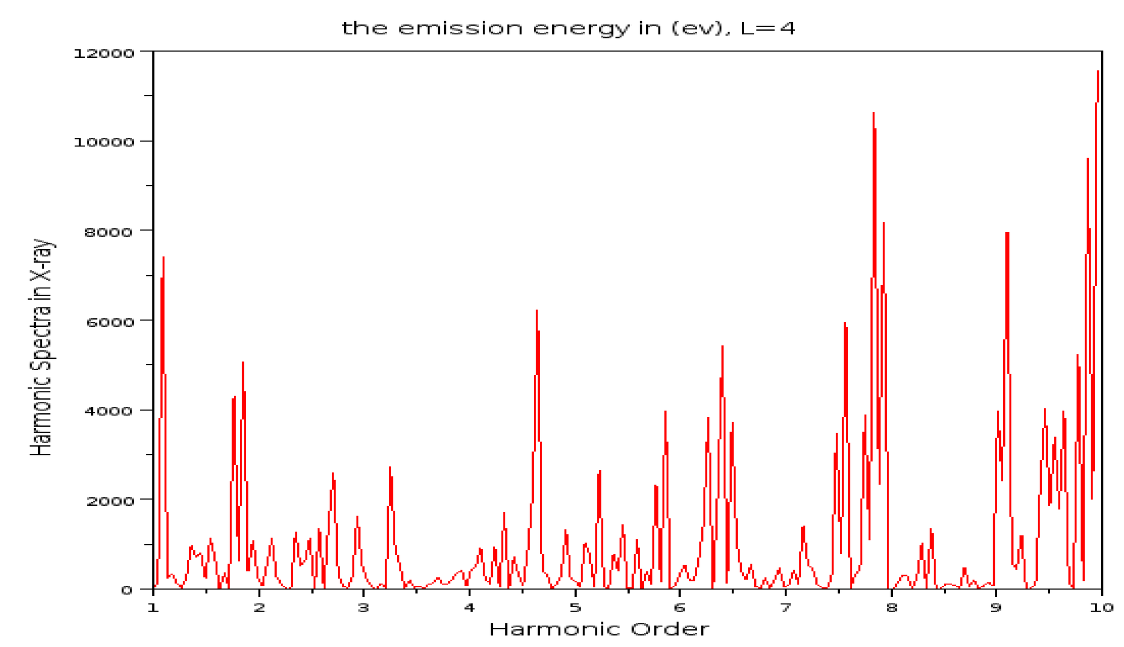

Figure 5: The emission spectra with spatial length L = 4.

>>From figure 5:
The electron was in a given level, when it interacts with the laser field, it gets accelerated to another level. This electron is then decelerated to a lower level when the field is reversed, the physical phenomenon corresponds to recombination, and this leads to it emitting light. This emission is represented by the peaks in the figure.

CONCLUSION

A quantum particle (Hydrogen atom) interacting with a Continuous femtosecond laser [3] has been considered and modeled with the Time Dependent Schrödinger Equation (TDSE).

-The TDSE has been numerically solved using FFT Split Operator method , thereby providing us with the time dependent wave function Ψ(x,t). The numerical code has been written in Scilab programming language.
-Using an arbitrary initial wave function, the X – Rays emission spectra have been obtained by Fourier Transforming the Dipole Acceleration originated from the Ehrenfest Theorem.

OUTLOOK

With all the theory and the numerical simulations we have learned here, we are eager to apply them on several open problems related to the HHG which is nowadays one of the hottest topic in the field of laser matter interaction.

REFERENCES

[1] Mendilyi Yohanna, "X-rays Emission from Atoms Driven by Ultrafast Lasers", Essay Thesis, AIMS – Senegal (2014),
[2]T. Brabec and F. Krausz, Rev.Mod.Phys. 72, 545 (2000),
[3] William.T.Silfvast, Laser fundamentals second edition, 1, 131 (1996).

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