Annual Summary Document

Year: 2020

Months: 16.10.2020 – 31.12.2020

Project Title: Plasma harmonics for diagnosing plasma and driving laser

Project Work Plan (according to the contract)

Stage: I. Theoretical study of the models describing the laser-plasma interaction and harmonics generation

Activities:

I.1. Study of the plasma mirror model for HHG and plasma dynamics, numerical programming in COMSOL and MATLAB

I.2. Project management

Cover Page:

Project title: Plasma harmonics for diagnosing plasma and driving laser
Project code: E_13/16.10.2020
Acronym: PHARDIPLAS

- **Group list (physicists, staff, postdocs, students);**

Physicist
Director of project: **conf.dr. Mihai STAFE**

Team members:
prof. dr. Niculae N. Pușcaș
Ș.l.dr. Georgiana Vasile
Ș.l.dr. Constantin Neguțu

PhD students:
Alexandru Enciu
Alexandru-Ferencz Filip
Răzvan Mihalcea

Staff: Ec. Ana-Maria Nicoleta Dragomir

- Specific scientific focus of group (state physics of subfield of focus and group's role);

The specific scientific focus of the group is related to the theoretical study of the models describing the laser-plasma interaction, to the theoretical study of the plasma mirror model for high harmonic generation (HHG) and plasma dynamics and to the numerical programming in COMSOL and MATLAB.

- Summary of accomplishments during the reporting period.

In the Phase 1 we carried a theoretical study on the models describing high harmonics generation (HHG) in plasmas (e.g. plasma mirror model) and plasma dynamics, and documented programming in COMSOL and MATLAB for HHG simulations.

The nonlinear optical process of harmonic generation in the gas can be described with a so called "three-step model". First, there is a tunnel ionizing of the gas atoms in the strong electric field of the laser pulse. Second, there is a subsequent acceleration of the free electrons along a trajectory given by the laser field and the atomic/ ionic potential. Third, there is the radiative recombination of the electron to the parent atom. HHG in gases leads to odd-order harmonics only, for symmetry reasons. Moreover, HHG in nanoparticle-containing gases can be described theoretically in the rigid sphere quantum formalism.

In contrast to the HHG in gases, HHG in dense plasmas leads to odd and even harmonics. HHG on dense plasma surfaces is usually described by the set of Lorentz-Maxwell equations for a pre-ionized collision-less plasma. The ions are assumed to form a fixed background density, and the electrons are fluidlike and driven by the laser field associated with the laser pulse. In the so-called oscillating mirror model, the electron density is treated as a rigid step function oscillating harmonically though a fixed ion background.

In the last part of the first Stage we realized a study of Particle-in-cell (PIC) simulation and COMSOL software. Particle-in-cell (PIC) simulation is an important numerical tool in plasma physics, providing a direct solution of the Lorentz-Maxwell equations for a system of charged particles interacting with the laser field. PIC simulations also enable prediction of the properties of surface harmonics. As well, we use finite-elements Newton method and a direct MUMPS solver implemented in COMSOL software to solve numerically the coupled non-linear wave equations for fundamental and harmonic radiations.

2. Scientific accomplishments – Results obtained during the reporting period.

According to activity A.I.1 of Stage 1, we carried a theoretical study on the models describing high harmonics generation (HHG) in plasmas (e.g. plasma mirror model) and plasma dynamics, and documented programming in COMSOL and MATLAB for HHG simulations.

2.1 Three steps model for HHG in gases

High order harmonics generation (HHG) in gases has been studied for three decades [1-4]. In most of the experiments, an intense femtosecond laser pulse is focused into a rare gas jet (helium or argon) and the transmitted light spectrum contains harmonics of the driving laser pulse. The nonlinear optical process of harmonic generation in the gas can be described with a so called "three-step model". First, there is a tunnel ionizing of the gas atoms in the strong electric field of the laser pulse. Second, there is a subsequent acceleration of the free electrons along a trajectory given by the laser field and the atomic/ ionic potential. Third, there is the radiative recombination of the electron to the parent atom. HHG in gases leads to odd-order harmonics only, for symmetry reasons.

HHG in nanoparticle- containing gases can be described theoretically in the rigid sphere quantum formalism [5]. The interaction of the of the atoms with the laser pulse field is described, in the single active electron approximation (constrained within a rigid sphere with $R \sim 6.7\ a_0$ radius) by solving the time-dependent Schrodinger equation [5]:

$$i\hbar \frac{\partial |\psi(x,t)\rangle}{\partial t} = \hat{H} |\psi(x,t)\rangle, \quad (1)$$

where $|\psi(x,t)\rangle$ is the full time-dependent wave function of the active electron acted upon by the laser field $E(t) = E_0(t)\sin(\omega_L t)$ at frequency ω_L. In Eq. (1) the Hamiltonian is written in the form $\hat{H} = \hat{H}_0 + \hbar cos\Omega_0(t) sin(\omega_L t)$, where $\hat{H}_0 = (\hbar^2 \hat{L}^2)/(2I)$ is the Hamiltonian of the atom (ion) in the absence of a laser field, $\hbar\Omega_0(t) = eRE_0(t)$, and $I = m_e R^2$ is the moment of inertia of the electron, and $\hat{L}^2$ is the angular momentum operator squared, whose eigenstates are the usual spherical harmonics $Y_{l,m}(\theta,\varphi) \rightarrow |l,m\rangle$, *l* being the orbital angular momentum, and *m* is the quantum number of the angular momentum projection.

It is convenient to write the full time-dependent wave function of the active electron at time t, as a linear combination of eigenstates of the laser-free Hamiltonian:

$$|\psi(x,t)\rangle = \sum_{l'=0}^{\infty} \sum_{m'=-l}^{l} a_{l',m'}(t) |l',m'\rangle \quad (2)$$

where $a_{l',m'}(t)$ are the expansion coefficients to be found by substitution into the time-dependent Schrodinger equation. Considering that $|\Lambda,m\rangle$ is the initial state for the highest-occupied atomic (ionic) orbital; according to the previous discussion, the laser field will couple only states with $m = m'$, finally one obtained the following equations:

$$\mathrm{i}\dot{a}_{\Lambda,m}(t) = \omega_\Lambda a_{\Lambda,m} + \Omega_0(t) b_{\Lambda,m} \sin(\omega_\mathrm{L} t) a_{\Lambda+1,m} \quad (3)$$

$$\mathrm{i}\dot{a}_{l>\Lambda,m}(t) = \omega_l a_{l,m} + \Omega_0(t) \sin(\omega_\mathrm{L} t)\left(b_{l-1,m} a_{l-1,m} + b_{l,m} a_{l+1,m}\right) \quad (4)$$

where $b_{l,m} = \sqrt{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+2)}}$. The set of differential equations (3-4) shows a ladder-like structure, so that any energy level is coupled to the two adjacent levels. This system can be numerically solved by using a MATLAB numerical routine.

2.2 HHG in plasmas

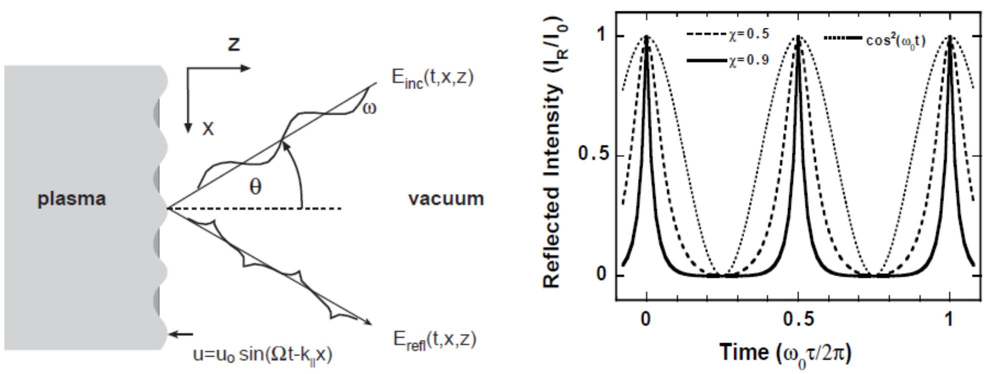
In contrast to the HHG in gases, HHG in dense plasmas leads to odd and even harmonics. HHG on dense plasma surfaces is usually described by the set of Lorentz- Maxwell equations for a pre-ionized collision-less plasma. The ions are assumed to form a fixed background density, and the electrons are fluidlike and driven by the laser field associated with the laser pulse. For linearly polarized laser pulses (along the y direction) impinging at normal incidence (along the x direction) on the plasma, the electromagnetic field can be represented by the vector potential $A_y(x,t)$. In this geometry, the electron momentum is $p_y = eA_y/c$. The wave equation for A_y, applying the Coulomb gauge, is:

$$\frac{1}{c^2}\frac{\partial^2 A_y}{\partial t^2} - \nabla^2 A_y = \frac{4\pi}{c} J_y \quad (5)$$

Here, the current density is related directly to the vector potential: $J_y = -n_e e v_y = \frac{n_e e^2}{mc}\frac{A_y}{\gamma}$, where γ is the relativistic factor. Thus, the problem of finding the harmonic content of the reflected light spectrum $|A_y(x,t)|^2$ reduces to determining the source term *Jy* responsible for the re-emitted radiation from the plasma surface. The electron density can be deduced from the continuity Euler equation describing the mass conservation: $\frac{\partial n_e}{\partial t} + \frac{\partial}{\partial x}\left(\frac{n_e p_x}{m\gamma}\right) = 0$.

2.3 Oscillating mirror model for HHG in plasmas

In contrast to the extended density profiles generated by nanosecond laser pulses, femtosecond laser-produced plasmas have little time to expand, so typical density scale lengths for a high-contrast laser are submicron [6,7]. During the interaction, the plasma surface can thus be represented to a good approximation by a simple step profile and assumed to be over-dense ($n_e \gg n_c$), so that it acts as a mirror reflecting the incident light in the specular direction. In the so-called oscillating mirror model, the electron density is treated as a rigid step function oscillating harmonically though a fixed ion background. In terms of the electron density, we can write $n_e = n_0 H(x - \xi(t))$, where H(x) is the Heaviside step function. We assume that the instantaneous mirror position has a harmonic variation in time: $\xi(t) = \xi_s \sin(\omega_L t)$



(a) (b)

Fig. 1. (a) Reflection of the incident laser pulse on a a plasma layer at the surface of a solid target. The darker area indicates the fixed ion background charge. (b) Train of attosecond light pulses obtained by reflecting a monochromatic wave (dotted curve) from an oscillating mirror. [7]

The reflected electric field is therefore emitted from a moving surface, and, omitting constant phase factors, can be approximated by $E_{refl} = E_{inc}\sin(\omega_L t_{ret})$, where $t_{ret} = t - \frac{\xi(t)}{c}$ is the retarded time at the observation point. Thus, the reflected anharmonic field is $E_{refl} = E_{inc}\sin\left(\frac{\omega_L t - \xi_s \sin(\omega_L t)}{c}\right)$. Fig. 1(a) presents the incident sinusoidal field and the distorted field reflected on the oscillating electron mirror at the plasma surface. Here, *u* describes the excursion of the electron surface along the normal z direction. Fig. 1(b) presents the time variation of the reflective wave intensity. One can see that, in the highly relativistic case ($\chi \sim \frac{\omega_L u_0}{c}$ =0.9), the full width at half maximum of the pulses corresponds to approximately 3 percent of the fundamental optical cycle.

2.4 PIC simulations

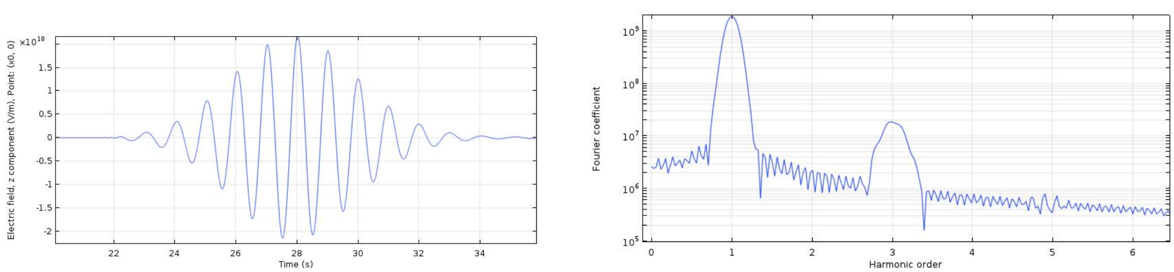
Particle-in-cell (PIC) simulation is an important numerical tool in plasma physics, providing a direct solution of the Lorentz-Maxwell equations for a system of charged particles interacting with the laser field. PIC simulations also enable prediction of the properties of surface harmonics [6]. To model HHG with a PIC code, it is necessary to choose a sufficiently small time-step to simulate the highest frequency of interest. Also, the simulation box must be large enough to prevent electrons from “escaping” the cell, which would inflict the overall charge neutrality of the plasma. Typically, this latter requirement is fulfilled if simulation region is of the order of a few laser wavelengths or several microns. These considerations lead to an overall computational effort of 10–20 CPU hours on a single-processor PC. Equivalent two- and three-dimensional runs with the same resolution remain a challenge even with substantial supercomputing resources, but useful information can be and is still gained with lower resolution.

2.5 COMSOL simulations

In the non-relativistic intensity regime, the microscopic and macroscopic properties of the plasmas relevant for the harmonics generation (real and imaginary refractive index, linear and non-linear susceptibility, real and imaginary electric conductivity of the plasma) are determined from the plasma hydrodynamics simulations. For “long” laser pulses (ns and ps), the stationary problem can be employed for study of HHG in plasma. The non-linear Maxwell equations describing the propagation of different harmonics (at frequency ω_q) within the plasma can be written as:

$$\nabla \times \left(\nabla \times \vec{E}_q\right) - k_q^2 \left(\varepsilon_r - \frac{i\sigma}{\omega_q \varepsilon_0}\right)\vec{E}_q = \omega_q{}^2 \mu_0 \vec{P}_{NL}(\omega_q) \tag{6}$$

where q index indicates the harmonic order, σ is the complex plasma conductivity, ε_r denotes the dielectric constant, and the non-linear polarization $\vec{P}_{NL}$ is dependent on q-th order susceptibility $\chi^{(q)}$. We use finite-elements Newton method and a direct MUMPS solver implemented in COMSOL software to solve numerically the coupled non-linear wave equations for fundamental and harmonic radiations.



(a) (b)

Fig. 2. (a) Time dependent output field for 10 fs incident laser pulse at 1064 nm wavelength ant 70 TW/cm^2 intensity. (b) Fourier transform of the time dependent output signal .

For the ultrashort fs pulses, the non-linear time dependent equation is used:

$$\nabla \times \left(\nabla \times \vec{E}\right) + \mu\sigma \frac{\partial \vec{E}}{\partial t} + \mu \frac{\partial}{\partial t}\left(\varepsilon_0 \frac{\partial \vec{E}}{\partial t} - \vec{P}\right) = 0 \tag{7}$$

where $\vec{P}$ has linear and nonlinear parts. In the time domain, the distorted output field is presented in Fig. 2(a). The Fourier transform of this field reveals the third harmonic radiation (Fig. 2(b)).

The output data of the COMSOL are stored in Excel worksheets. These worksheets act both as data storage and as feed-in for a successive program in MATLAB that processes these data to calculate additional characteristic measures of the non-linear process.

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