Project Title: Nonlinear Drude plasma model for ultra-short pulse simulation

Abstract:

The goal of this project is to implement a program module which calculates the current density in a plasma driven by a strong femtosecond optical pulse. The current contribution from the ions is to be neglected (due to the very fast time scale), and the electron current density is to be calculated in the nonlinear Drude approximation. The module is meant to become a component of the Optical Pulse Propagator Toolkit.

The further aim of the project is to provide an opportunity for the team member(s) to a) learn the background of femtosecond light filamentation physics and b) acquire basic experience with computer simulations in this area.

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1. Motivation

Computer modeling of ultrashort (femtosecond) optical pulses interacting with gaseous and condensed media has been very important for the extreme nonlinear optics over more than a decade.

There is something that can be called a "standard model" to describe the interaction between the femtosecond optical pulse and a nonlinear dispersive medium. The effects included are: chromatic dispersion and frequency-dependent losses, Kerr effect (self-focusing), Stimulated Raman effect (self-focusing with memory), multiphoton ionization at high intensities ($10^{18}\mathrm{W/m^2}$), and interaction with the generated plasma.

The interaction with plasma is normally described as a Drude model, where ions are neglected completely (too heavy to move on the fast time scale), and electrons are described as an effective ensemble that suffers damping of the average velocity while driven by the electric field of the optical pulse.

Note that, among others, this approximation neglects the magnetic component of the Lorentz force. The rationale for this is that the latter is much weaker than the electric part.

The nonlinear Drude model includes the magnetic field effect, and leads (as the attribute indicates) to nonlinear effects in all orders (a fundamental frequency generates response at harmonic frequencies). Experiments with metallic nanoparticle arrays in which second harmonic radiation is generated have been recently described in terms of the nonlinear Drude model coupled to Maxwell's equation time-domain solvers.

In the femtosecond pulse community the current belief is still that inclusion of nonlinearity into the Drude model is not necessary. However, a recent experiment in which dense plasma "amplifies" third harmonic generation by two orders of magnitude indicates that the current model everybody uses may not be complete or sufficient.

One potential explanation can be the nonlinearity in the plasma response. The goal of this project is to create a simulator module that in turn allows us to study this exciting possibility.

2. Physical model description

A. *Drude model for plasma*

Let $\vec{E}(t)$ represent the electric field of an optical pulse at a fixed spatial point. Further, let $\rho(t)$ be the number density of free electron at this point. This may in general be a function of time, as the optical field may be strong enough to ionize atoms or molecules and the plasma density ρ may exhibit strong increase within the femtosecond pulse duration. Strictly speaking electrons also recombine, but this is usually neglected on this timescale. However, what can't be neglected is collisions: Their effect is included as a phenomenological velocity damping term characterized by the "collision time" τ:

$$\partial_t \vec{v}(t) = \frac{e}{m}\vec{E}(t) - \vec{v}(t)/\tau \tag{1}$$

and the current density is simply a product of plasma density and the ensemble velocity:

$$\vec{j}(t) = e\rho(t)\vec{v}(t) \tag{2}$$

The current density calculated this way appears on the RHS of the optical field propagation equation. If we consider plasma density ρ as given, it is clear that the Drude model response is linear; It manifests itself as a loss and change of the index of refraction. The latter is negative and causes defocusing of the optical field. This is crucial for the dynamics of femtosecond light filaments in gaseous media.

B. *Nonlinear Drude model*

The "only" difference from the linear version is that the complete Lorentz force is included:

$$\partial_t \vec{v}(t) = \frac{e}{m}\left[\vec{E}(t) + \vec{v} \times \vec{B}(t)\right] - \vec{v}(t)/\tau \tag{3}$$

In the femtosecond pulse, the velocity is non-relativistic and the magnetic force is small compared to the electric one. Thus, one can neglect it in the zero approximation, and the velocity will, roughly speaking, oscillate with the same frequency as the driving field (exactly as in the linear Drude model). Then this zero approximation can be fed into the magnetic term velocity to calculate the next correction. In this term we have two quantities that oscillate at the fundamental frequency. Consequently a component will appear that oscillates at the second harmonic frequency. In the same fashion, higher harmonics will be generated. Appearance of new frequencies is a manifestation of the nonlinearity of this version of the Drude model.

The current density is obtained as a sum over contributions from electrons liberated from the neutrals (atoms, molecules) at a given time:

$$\vec{j}(t) = e\int_{-\infty}^{t} V(t, t_0)\dot{\rho}(t_0)dt_0 \tag{4}$$

where $V(t, t_0)$ represents the solution of Eq. 3 for the electron "born" at time t_0.

This equations reduces to the linear Drude when the magnetic force is neglected. However, once B is included, we have to deal with the integral over t_0 for each time t we need to calculate the current density for. This is computationally significantly more intensive than the linear Drude problem. We will need to perform these calculations at every spatial point in our computational domain and at every propagation step. Thus, the speed is crucial here: we need a *fast algorithm.*

C. *Nonlinear effects captured by the model*

Closer inspection reveals that the second harmonic frequency component of the electron velocity oscillates along the direction of the pulse propagation. As such, it will not contribute to the radiation field. However, the third harmonic component oscillates in the same direction as the electric field and it will create third-harmonic radiation. This is the effect we are after. Our goal is to find out if nonlinear Drude model can explain at least a portion of higher-harmonic radiation generated by femtosecond pulses in relatively dense plasma.

3. Task specification

Task One:
The task one is to come up with an algorithm and implement a straightforward, brute-force-approach function that calculates the current density in the nonlinear Drude model approximation according to the equations (3,4) above.

There will be several inputs this function will accept (we will figure out the exact function signature at the start of the project):
The plasma density $\rho(t)$, the driving electric field $E(t)$, (optional) driving magnetic field $B(t)$, will be all sampled on an equidistant temporal grid, and the function will receive pointers to these arrays. If magnetic field is not given, it will be calculated (within the function) from the electric field as if in the plane wave propagating in a z-direction. For performance reasons, no memory allocations will be done within the function, and we will assume the arrays were allocated reasonably "from outside." However, as part of this first task, we need to determine if the temporal grids that are typical in femtosecond pulse simulations have sufficient resolutions, and design the solution strategy with this in mind.

Output is to be placed in a provided array and should represent the the current density $j(t)$.

Set of sample inputs will be provided, so that one can work and debug the implementation without the need of the complete simulator. At present, we have no functionality against which the product can be tested, so detailed testing (including writing corresponding program(s)) will have to be done as well.

Task Two:
Task two, if time permits, will be to tune the algorithm to obtain good performance. As a part of this sub-task, we will explore possibilities to introduce further approximations, especially if it turns out that the current calculation is numerically too expensive.

Task Three:
Most likely for the work following the School: The program will be linked with the UPPE simulator, and used to simulate the experiment described in the paper by Suntsov. Also at this stage, we will need to examine the physical regimes (characterized mainly by plasma densities and light intensities) where the inclusion of the nonlinearity in the model becomes important.

Literature:

Motivation paper on enhancement of third-harmonic in plasma filament:
S. Suntsov, D. Abdollahpour, D. G. Papazoglou, and S. Tzortzakis, *Efficient third-harmonic generation through tailored IR femtosecond laser pulse filamentation in air*, Opt. Express 17, 3190-3195 (2009)

Broader context (this is a long review, no need to read everything):
A. Couairon, A. Mysyrowicz, *Femtosecond filamentation in transparent media*, Physics Reports 441, 47-189 (2007)

Overview of pulse propagation equations and medium models used in the femto-second area:
M. Kolesik, J. V. Moloney, *Nonlinear optical pulse propagation simulation: From Maxwell's to unidirectional equations* Physical Review E 70 (2004) 036604

Simulation of thrid-harmonic in more detail:
M. Kolesik, E.M. Wright, A. Becker, J.V. Moloney, *Simulation of third-harmonic and supercontinuum generation for femtosecond pulses in air* Appl. Phys. B 85, 531538 (2006)