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REPORT

from Mr Richard TAÏEB, Directeur de Recherches au CNRS on the PhD manuscript of:

Mr Jan VABEK

on:

" Multiscale approach to the description of high-harmonics generation in gases"

Background of the work :

The PhD work of Mr Jan VABEK deals with the theoretical study of High Order Harmonic Generation (HHG) in gas and the interplay between microscopic, i.e. atomic, and macroscopic, i.e. field propagation, effects. This work was performed between two theoretical groups in CELIA, Université de Bordeaux, France and the Czech Technical University in Prague, Czech Republic, in close collaboration with experimental groups either in CELIA or at ELI-Alps, Szeged, Hungary. To this aim, Mr Vabek developed both analytical tools and heavy numerical machinery to propagate the Time Dependent Schrödinger Equation, for the microscopic part and the Maxwell Equations for the macroscopic response, respectively, in a coupled way. The goal of this manuscript is to exhibit how a better knowledge of the macroscopic behavior of the HHG, an aspect which is often not considered, restricting the study of HHG to the atomic response, allows us to have a better control on the harmonic emission either in a thin gas target or in a pre-ionized long atomic cell.

One of the originalities of this PhD thesis is the constant intent to relate the theoretical results obtained by Mr Vabek with experimental results and the agreement is rather impressive. This work is perfect line of many developments from the CELIA group, where, for the last 10 years, they found many ways to optimize HHG emission. Furthermore, he brings new physical insights of the results obtained numerically by its combined code.

Content:

This PhD manuscript contains three parts corresponding to the different scales of the problem, i.e microscopic in Part I, macroscopic in Part II and all the numerical aspects in Part III, which are essential to grab the amount of work performed during this PhD. They are preceded by an introduction and a preliminary chapter.

The manuscript starts with an introduction where the HHG process and its different aspects are presented and where Mr Vabek explains the strategy and the developments contained in his

manuscript. In the meantime, he points out a crucial feature, namely the definition of ionization, as it is not straightforward to compute it rigorously and as it is essential in the change of the index of the medium affecting the propagation of the fields and the phase-matching of HHG.

In the preliminary chapter, all basic concepts are explained from the microscopic point of view (3-step models, ionization, ...) to the macroscopic effects (propagation of the fields via the Maxwell Equations, or the different impacts between the longitudinal and the transverse components of the IR and the XUV of the non-linear medium).

The first Part of this manuscript concentrates on the atomic response in HHG process. Based on quantum dynamics principles and, for example its invariance in terms of field gauge, Mr Vabek presents the different models that are used throughout this thesis. One chapter is dedicated to find a more rigorous way to define the ionization of an atom. After presenting different models to compute or approximate atomic ionization for various regimes of frequency and intensity of the external field, a definition of the ionization is derived in terms of invariant energy and stabilized spectrum by a change of Hamiltonian. Examples of the "new definition" of ionization are given at the end of this chapter for the one, two photon or tunnel regimes.

In the second Part of this manuscript, Mr Vabek deals with the macroscopic effects of HHG and will consider two different cases for the generating medium, i.e. a thin target, for which the important parameter is its position with respect to the IR laser focus or a dense cell, which is preionized by a discharge.

In chapter 4, the wave equation is derived using the transformation from time to frequency in the Maxwell Equation and the link between the emitted microscopic dipole and its macroscopic counterpart.

In chapter 5, the case of the thin target is presented, where transverse aspect of the generation is dominant. Thus, an original way of treating the beams propagation in terms of combination of curvatures is presented and used. Then, a comparison between three atomic dipole modeling is studied and its influence on the HHG spectra for three harmonic order is shown and demonstrated that there is a selectivity both on focusing and propagation properties of the harmonics, when varying the jet position. This dependency also translates in modifications of cut-off positions and transmittance of the harmonics. It also shows that the Strang field Approximation is in accordance to the full solution of the TDSE. Finally, after comparison with experimental results, exhibiting a good agreement, the chapter deals with temporal aspects of HHG, when changing the jet position and showing that the "macroscopic averaging" smoothed the time profile of the generation.

In chapter 6, Mr Vabek studies HHG in long gas cell where an "important" number of free electrons are generated by a discharge before the arrival of the strong IR laser field responsible for HHG. In these conditions, the decoupling of the longitudinal and transverse effects are not anymore possible. Before giving numerical examples, all aspects of the propagation and of the non-linear aspects are reviewed in particular the link between the microscopic dipole and the source term in the Maxwell Equations. With all in hands, comparison with experimental results and the simulations is performed and analyzed for different conditions of ionization and pressure in the cell. While the agreement is rather good, the discrepancies were appraised in terms of fluctuations of the experimental conditions. The chapter end with a fine analysis of the focalization, temporal and fluence properties of the HHG beam.

The third part of the manuscript describes all the numerical aspects used to produce the results of Part I and II. First, it gives a wide review of almost all ways of solving the TDSE equations for an

atom interacting with an intense short laser pulse and how to compute ionization. Then, the CUPRAD algorithm to propagate the fields is presented and how it is coupled with the solution of the TDSE.

Finally, a conclusion of the results as well as numerous perspectives both from the physics or the numerical point of view of this work are presented.

The manuscript is complemented with an abundant bibliography (more than 300 references!) and multiple annexes containing very useful informations.

Comments:

When reading this manuscript, I was impressed by the care and the precision that Mr Vabek took to present both the methodology he used and the results he obtained. The manuscript is very well structured and each subpart has a real meaning. Even though, the manuscript gives all the details needed to understand the reasoning and the analysis of the results, Mr Vabek stays focused to present in very clear and pedagogical way the physics that is contained in the processes at play. I found very important to relate his results to "real" experiments not only to reproduce the results but to give more informations on the main mechanisms.

This manuscript contains a wealth of very high-quality results, which translates in 3 peer-reviewed articles in excellent review, another already submitted and probably more to come. While the manuscript needs a lot of attention from the reader, as it contains lots of informations, it is pleasant and all physics ideas are clearly presented.

The works contained in this manuscript clearly shows that Mr Vabek masters is subject both from the conceptual, physics and numerical aspects. He was very precise in testing all hypothesis and extracting all useful informations.

I think that he has demonstrated his ability in pursuing a bright and autonomous scientific activity.

Therefore, I believe that all the works presented in this manuscript form an excellent PhD Thesis and I give my firm approval, with no reserve, to Mr Jan VABEK to defend it in front of a jury and recommend awarding degree after successful defense.

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