Centre Lasers Intenses et Applications

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Report on Short Visit Grant SILMI-5351
Hosted by Prof. Viorica Florescu at Bucharest-Magurele, Romania
From January 21 to January 27 2013

Title of the project: Above-threshold ionization of hydrogen and hydrogen-like ions in short X-ray pulses

1 - Purpose of the visit

Since two years, our collaboration with Profs. Viorica Florescu and Mihai Dondera has focused on the problem of hydrogen atom and hydrogenic ions submitted to X-ray intense field. The problem is related to the rapid development of free electron lasers which already provides intense field in the soft X-ray region. This opens the door for the study of non-linear processes at ultra-short wavelength and pulse duration, i.e., a field which has received little attention until now. Two approaches are explored, in the first one we calculate generalized differential and total cross sections based on second-order perturbation theory for the electron interaction with a monochromatic plane wave, with the $\mathbf{A}^2$ and $\mathbf{A}\cdot\mathbf{P}$ contributions treated exactly. In the second approach, we solve the time-dependent Schrödinger equation (TDSE) for a pulsed plane wave using a spectral approach and a basis of L^2-integrable B-spline functions. Retardation effects are included up to $O(1/c)$, they induce extra terms

forcing the resolution of the TDSE in a three dimensional space. Relativistic effects [of $O(1/c^2)$] are fully neglected.

The objective of the short stay in Bucharest is twofold; first we plan to investigate the case of two-photon ionization of hydrogen in the threshold region with two X-ray fields of different frequencies (two colors), second we like to explore the case of ultra-short pulses, with a rapidly varying temporal envelope, where we expect relativistic corrections to be non negligible.

2 - Description of the work carried out during the visit

During the visit we have mainly investigated the problem of X-ray two-color photon ionization of hydrogen and hydrogen like ions. The idea is to study a two-color process where one X-ray photon with energy ω_1 is absorbed while another photon, of energy ω_2 (with $\omega_2 < \omega_1$) is emitted. The difference ω_1-ω_2 is slightly greater than the ionization potential of the atom or ion considered, therefore the emitted electron has a low energy. The region of the threshold is of particular interest since we expect a larger two-photon ionization rate, it will be also interesting to investigate the retardation effects on the emitted electron angular distributions. The figure 1 shows the schema of the two-photon transition, with the two paths leading to the same final state |F>. Both paths involve the absorption of photon ω_1 and the emission of photon ω_2, but with a different sequence.

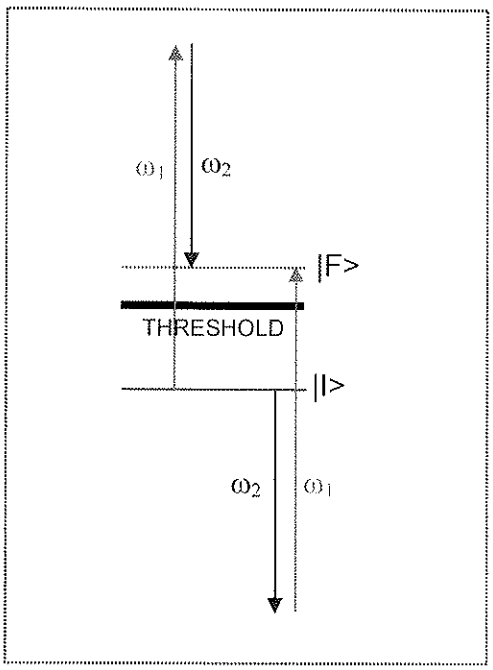

Figure 1. Two-color two-photon ionization with photons of energy ω_1 and ω_2. |I> is the initial state, |F> is the final continuum state, located above the threshold. The figure shows the two paths associated to the two-photon transition between |I> and |F>.

Concerning the case of ultrashort pulse we have discussed the problem similar to the one exposed above but with $\omega_1 = \omega_2$. Thus we consider one-color two-photon ionization where the laser bandwidth, roughly given by $2\pi/T$ where T is the pulse duration, is larger than the ionization threshold. In this case we expect that, due to the laser bandwidth, the states above and below the ionization threshold will be populated. We have also discussed, in this context, the influence of the temporal pulse shape on retardation effects.

3 - Description of main results obtained

Concerning two-color two-photon ionization we have first investigated this process using the TDSE approach (see M. Dondera and H. Bachau, Phys. Rev. A **85** (2012) 013423), generalized to the two-color case. We have analyzed the preliminary results during the visit. We have investigated the cases of hydrogen and hydrogenic ion C^{5+}. Figure 2 shows the case of C^{5+}, three values of the ω_1 photon have been investigated; 110 au, 220 au and 440 au. The value ω_1 - ω_2 is fixed at 23 au, and the corresponding field intensities are fixed at 3.51 10^{16} W/cm^2. The figure shows that, has expected, one-photon absorption dominates (see the couple of peaks close to 80, 200 and 400 au). The two-color two-photon process leads to the structures close to threshold (see the three peaks close to the energy zero in figure 2).

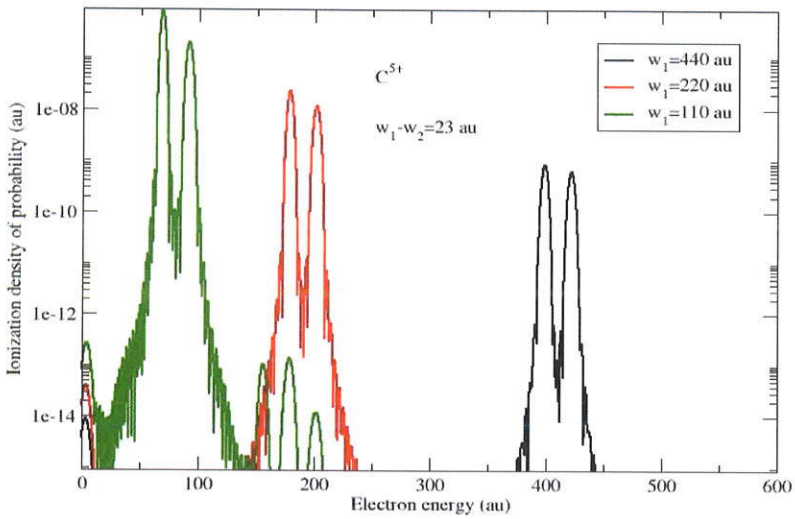

Figure 2. Two-color two-photon ionization of C^{5+}, TDSE calculations. Three cases are considered, the values of the photon energies are indicated in the figure.

Several questions arise;

- the relative contribution of the two paths shown in figure 1 in two-photon ionization
- the scaling law in ω_1 of the two-photon process, compared to one-photon ionization

In order to answer the two questions it has been decided to investigate the process in second order perturbation theory (see V. Florescu, O. Budriga and H. Bachau, Phys. Rev. A **86** (2012) 033413). Also we plan to pursue this work with the study of angular distributions, which have been shown in precedent works to be sensitive to retardation effects.

Concerning the case of ultrashort pulse mentioned at the end of section 1, i.e., one-color two-photon ionization in the threshold region, it is in fact a particular case of the two-color problem mentioned above (setting $\omega_1 = \omega_2$). Therefore the extension of the TDSE approach to this case is obvious. Nevertheless, it is well known that the resolution of the TDSE has severe limitations in the threshold region. Indeed, since the problem is solved "in a box" of finite radial dimension, the high Rydberg states and low energy continuum are not well represented. This raises the question of the convergence of the calculations in the threshold region. This convergence may be numerically checked by varying the "box" dimension. We have also decided to develop a time-dependent second-order perturbative approach, including the analytical expression on the wave-functions in the threshold region, in order to compare with TDSE results.

4 - Future collaboration with the host

The support of the ESF Research Networking Program SILMI and COST Actions (CUSPFEL until May 2012 or the newly accepted XLIC Action) are of crucial importance for the continuation of the collaboration. Also we have discussed the possibility to apply for bilateral programs between France and Romania, like the program "Brancusi" or the program "Blanc International" of the Agence Nationale de la Recherche.

5 - Projected publications/articles

The TDSE resolution of the two-color two-photon ionization problem is well advanced and we plan to publish one or several papers during 2013.

6 - Visit of the laser department of the National Institute for Laser, Plasma and Radiation Physics (INFLPR)

I have been invited by the Head of the laser department of the INFLPR, Dr. Viorica Stancalie, to visit the various laboratories and lasers facilities of the institute. I had very interesting and fruitful discussions with the researchers on charge of the experiments.

7 - Conclusion

This short stay at Bucharest-Magurele has been an opportunity to strengthen the collaboration with Viorica Florescu, Mihai Dondera and Olimpia Budriga, and to meet other collaborators. We have been able to progress in our present scientific work and to give clear directions for the continuation of the collaboration. I am fully satisfied by my visit at the department of Physics and Centre for Advanced Quantum Physics of the University of Bucharest.

Monday 28th January 2013

Henri Bachau

Directeur de Recherche au CNRS