SCIENTIFIC REPORT

SHORT VISIT GRANT (Ref. No. 4203)

TITLE: ULTRAFAST DYNAMICS of MULTICHANNEL CONTINUA and AUTOIONIZING STATES

The purpose of the short visit to CELIA, was to collaborate closely with Dr. H. Bachau on a theoretical /computational study of the ultrafast dynamics of multi-channel continua and autoionizing (AI) states. The project commenced in fall 2010 and prior to the applicant's ESF-funded short visit at CELIA, it had reached a stage at which a critical evaluation of implemented computational procedures was necessary as well as the development of suitable theoretical /computational techniques for studying specifically the ultrafast dynamics of AI states.

The research work was split in two different tasks: (1) completing the development of a two-photon two-color pump-probe TDSE code for the study of the electronic correlation dynamics of the Helium multichannel continuum and assessing its performance and output ; (2) formulating a theoretical approach and its computational implementation for the study of electronic correlation dynamics in Helium AI states. Work has been carried out on both directions with more emphasis placed on task (1) as it was at a more advanced stage and was expected to yield the first numerical results to corroborate earlier preliminary evidence that the devised pump-probe scheme was suitable for monitoring the time evolution of electronic correlation. As part of task (2), the theoretical /computational approach to extract information on the electronic correlation dynamics of an AI state from the time-dependent two-electron wavefunction at the end of the pump-probe interaction was developed. The crucial differences with the multichannel continuum states were identified and the approach to address them correctly was formulated. The main steps of the computational implementation of this approach were also outlined.

The main results obtained were: (1) The first numerical results for two-photon two-color ionization of He by a pair of mutually delayed pulses (pump pulse followed by the probe one) as a function of the delay between the pulses. The ionization results in the {1sks J=0 and 1skd J=2} continua confirmed that it is indeed possible to follow the time-evolution of the electronic correlation in the multichannel continuum above the n=2 He ionization threshold by the pump-probe scheme we have implemented. However, it is now necessary to carry out a systematic study of the pump-probe process in order to identify, by a careful analysis of the results, which details of the correlation dynamics can be unambiguously retrieved by the implemented pump-probe scheme. It is also necessary to carry out a numerical convergence study. These time-consuming tasks could not be completed within the limited duration of the short-visit and will be the subject of the continuing collaborative effort in the following months. (2) A theoretical formulation and a corresponding computational scheme for the study of electronic correlation in certain AI states of He has been detailed. In particular, we were able to identify which aspects of the approach employed for the study of the multichannel continuum need to be modified due to the presence of bound interacting channels in the case of AI states. We have detailed the

pertaining modifications as a first step towards implementing the computational scheme, a process that will be continued in close collaboration in the following months.

The collaboration between the two parties (Dr. A. Lyras and Dr. H. Bachau) will be continued in a systematic way in the following months, since the project is complex and demanding, as already explained above. The long-term research strategy already outlined during the short visit will be reassessed periodically on the basis of accumulated results and adjusted appropriately, if necessary.

It is reasonably expected, on the basis of the progress achieved so far, that before the end of 2011 a paper on our results for the correlation dynamics of a multichannel continuum will be submitted for publication, citing the funding by the ESF.