Project Title: Computational pump-probe spectroscopy involving X-ray laser fields

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Type of Project: COMPUTATIONAL/THEORETICAL

Helpful existing knowledge: A good knowledge of quantum mechanics is essential, whereas knowledge of computational methods is desirable.

Funding status: No specific funding

Project Description

Over the last 20 years, great strides have been made in our understanding of ultra-fast atomic dynamics and we can now measure processes on the timescale it takes an electron "to go round an atom". This progress was recognised in 2023 by the award of the Nobel Prize in Physics to researchers instrumental in developing the technology of attosecond light pulses [1]. Experiment needs to be complemented by theory: our R-matrix codes for time-dependent processes [2] calculated a photoionization time delay of 10 attosecond (10^{-18} s) between the emission of a 2s and of a 2p electron in Ne [3]. This interplay between world-leading theory and experiment is critical in the progress achieved in the last two decades.

The development of X-ray free-electron laser facilities has opened up research into the dynamics of so-called hollow atoms with inner-shell vacancies. As the photon energy of X-ray laser light is much higher than standard visible light lasers, tightly bound inner-shell electrons can be removed from atoms. The sudden removal changes the central charge seen by the outer electrons, and they will therefore start to 'wiggle'. However, no one really knows how they do so, and how best to observe this motion. New theory is thus needed, both to predict and to interpret experimental observations.

We can create this new method by combining our R-matrix codes through density-matrix technology. The X-ray laser field leaves the residual ion in a coherent superposition of states, which can be described through a so-called density matrix. We then investigate the states separately, and use the correlations captured within the density matrix to reconstruct the overall dynamics. This technique has now been applied successfully within R-matrix theory [4].

In this project, we will investigate the dynamics in Ne^+ ions following emission of a core 1s electron from Ne. Neon provides the most accessible system to investigate the dynamics of atoms with an inner-shell vacancy, and is also used frequently in experimental investigations. Initially, we will investigate the fundamental characteristics of the dynamics. We will subsequently look at the importance of different approximations to the overall description.

Skills gained by student

The project will allow to develop a range of highly valuable skills. The student will gain great understanding of fundamental quantum mechanics as well as advanced computational techniques. The project may offer substantial opportunities to engage with experimental research at free-electron laser facilities. The project will also see students develop excellent communication skills.

Useful references

[1] Nobel Prize Committee, Scientific Background to the Nobel Prize 2023

[2] A.C. Brown et al, Comp. Phys. Commun. 250, 107062 (2020)
[3] L.R. Moore et al, Phys. Rev. A 84, 061404(R) (2011)

[4] H. Lavery, in preparation.