Centre for
Theoretical Atomic, Molecular and Optical Physics
CTAMOP
Queen's University Belfast

Ph.D. Project 2019-2022

Attosecond Spin-Orbit Spectroscopy

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State of the art and motivations

Taking pictures of fast moving objects requires short pulses of light: instead of opening and closing a camera shutter at speeds beyond their mechanical capability, photographers in the 1960s hit on the idea of leaving their cameras 'open' in a dark room. They would then switch the lights on and off at the moment that, say, a bullet passed in front of the camera, allowing them to capture a still image of a fast moving object.

Similar schemes are used every day in physics labs: with recent improvements in laser technology, experimentalists are routinely able to generate laser pulses which are mere attoseconds (1 as $= 1 \times 10^{-18}$s) in duration. This has facilitated several incredible experiments which have been able to 'photograph' (or even 'video') electron dynamics which evolve on the attosecond scale [1].

One exciting application of these techologogies has been to probe the evolution of atomic systems driven by 'weird' quantum effects: correlated electron-hole dynamics for instance. As metrological techniques have become more and more sensitive, it has been possible even to elucidate more subtle quantum effects such as spin-orbit coupling which causes splitting of atomic states and associated dynamics. As far back as 2011, experimentalists were able to resolve the attosecond-scale interference effect between two spin-orbit split states in Krypton [2]. Unfortunately, as the experimental techniques have marched onwards, theoretical treatments have lagged behind. However, now with recent developments made at Queen's, we are finally able to support and even lead experiment with our world-leading computer code for modelling laser-atom dynamics: RMT.

Objectives & Methodology

The purpose of this project will be to use newly developed capability in the RMT code to address state-of-the-art experimental schemes for atto-scale dynamics in atoms, ions and perhaps even molecules. Recent capability expansions now allow us to model arbitrarily polarised laser pulses and, importantly for this project, relativistic effects in the description of the atomic structure and dynamics. **No other method exists to address these problems** so we are in a unique position to lead the field. The project will begin with an orientation to the computer code and the key physics, but thereafter a vast realm of uncharted science awaits your exploration.

Collaborations

We are managing partners in the UK-AMOR consortium: a high-end computing collaboration focussed on atomic, molecular and optical physics comprising more than thirty researchers across the UK. As part of this project you will spend time working with other members of the consoritum whose research is into traditional atomic physics, molecular dynamics and ultracold chemistry.

Required skills

.5 The successful candidate should have a solid grounding in mathematics and physics, with a firm grasp of quantum mechanics. A decent level of programming ability, in particular using Fortran and/or parallel computing techniques, is desirable, but training in these aspects of the project will be provided.

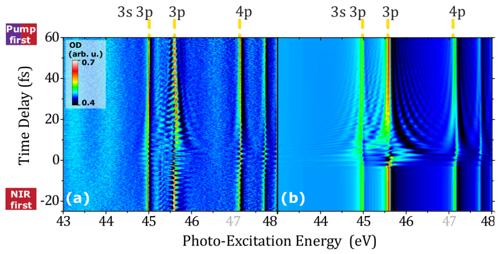

Fig. 1: Absorption spectrogram of neon showing the coupled dynamics of core- ($2s2p^6np$) and doubly-excited ($2s^22p^43s3p$) states in neon as measured in experiment (left) and calculated using the R-matrix with time-dependence codes at Queen's (right) (adapted from [3]).

Further information

Queen's University Belfast hosts an active group in the study of ultrafast processes using R-matrix theory. This group presently comprises 2 academic staff and 2 Ph.D. students and 2 post-doctoral research assistants. The group has a good record of Ph.D. student and PDRA success, both during their studies and further career.

The group is one of the leading users of massively parallel computing in the UK. Through development of our own software, researchers trained in CTAMOP have gone on to become industry leaders in the development and exploitation of parallel software.

For further information, please contact Dr Andrew Brown: andrew.brown@qub.ac.uk.

References

[1] F. Krausz and M. I. Stockman, Nat. Photon., **8**, 205 (2014)

[2] A. Wirth *et al.* Science, **334**, 195 (2011)

[3] T. Ding *et al*, Opt. Lett. **41**, 709 (2016)