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

PH.D. PROJECT 2020-2023

Attoclock: timing photoionization on the sub-femtosecond timescale

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State of the art and motivations

The development of ultra-short light pulses and associated measurement techniques have greatly enhanced the level of detail with which fundamental processes in atomic and molecular physics can be investigated. One of the key questions that is being asked at the moment is the origin of time delays in photoionization. When electrons in different shells are emitted after photoabsorption, they appear with a slightly different phase. This different phase can be interpreted as a time delay, and, hence, it appears as if the electrons absorb the photon at slightly different times [**?**]. When a short circularly polarised light pulse is used to eject the electrons, we can use the difference in angle between the peak of the ejected-electron density and the orientation at peak electric field as a measure of the apparent time delay for photoionization [**?**].

The physics of these time delays is still posing questions to scientists. Many studies of the time delays have used relatively simple atomic models. A standard approximation is that only the ejected electron is taken into account. In other cases, the physics is described by treating the system as a single-electron system within a model potential. However, the physics involved in photoionization is more complicated than this. When an outer electron is ejected, all the other electrons will notice the absence of this electron, and rearrange themselves. A full description of the physics will thus need to account for the full multi-electron dynamics in the system, and only a few methods are available for the accurate description of multi-electron systems in short light pulses.

One of the most advanced methods for the description of multi-electron systems in arbitrary light fields is the R-matrix with time-dependence method (RMT), which has been developed in Belfast over the last 12 years. In recent years, we have made substantial developments to the code, including its application to atoms in arbitrarily polarised light fields, and its application to systems with notable (relativistic) spin-orbit effects. With these developments in place, QUB is now well-placed to apply the RMT codes to key questions on time delays in photoionization.

Objectives & Methodology

In this project we will be using the RMT codes to study photoionization time delays in a range of systems [**?**]. The RMT codes are regarded as one of the leading codes for the description of the interactions between light and atoms. They have been designed to make efficient use of the largest computational facilities available. Typical calculations for linearly polarised light

would use around 500 cores, but for arbitrarily polarised light typical calculations may employ over 10000 cores. The codes are now well established, so although there is no need to become too involved with code development, the project offers significant opportunities to learn about massively parallel computing.

In the first instance, we will be using the RMT codes to investigate attosecond time delays in light atomic systems, such as Ne or Ar. We will be investigating how these time delays depend on the amount of atomic structure included in the calculations, and on the laser fields included in the experiment. Once we have established good understanding for these light atoms, we will continue the investigations for heavier atomic systems, where the influence of relativistic effects, such as the spin-orbit interaction, can no longer be neglected.

Collaborations

The RMT codes have been developed in collaboration with the Open University, where researchers are interested in its application to molecular systems. Ongoing development will likely also involve the Charles University in Prague. Over the last years, we have increasingly been involved with external collaborations, including leading research centers in Germany, including the Max-Planck Institute in Heidelberg and the Max-Born-Institute in Berlin. We are also planning new collaborations with the theoretical AMO group at University College London.

Required skills

Typical skills required are those acquired by a first-class Masters-level graduate in Mathematics and/or Physics. A good core understanding of Quantum Mechanics is important. Good computational skills would be beneficial, but are not essential.

Further information

For further information, please do not hesitate to contact Prof. Hugo van der Hart in his office, room 01.002 in Old Physics, or by email, h.vanderhart@qub.ac.uk

References

[1] M. Schultze *et al*, Science **328**, 1658 (2010).

[2] A.N. Pfeiffer *et al*, Nature Physics **8**, 76 (2012).

[3] A.C. Brown *et al*, Computer Physics Communications, in press (2020); https://arxiv.org/abs/1905.06156