Project Title: Mapping the transition from photo-ionisation to strong-field ionisation.

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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: Awaiting internal funding

Project Description

The 2023 Nobel Prize in physics was awarded in the field of Attoscience[1]. One attosecond is 10^{-18}s, and it is on this timescale that electrons move in response to light in atoms and molecules. Understanding and controlling this motion with ultrashort laser pulses will be key to new technologies such as ultrafast electronic circuitry, and novel solar cells. For now, scientists are still grappling with understanding the rich dynamics of electrons at the fundamental level[2].

At Queen's, we are driving this effort with the world-leading R-matrix with time-dependence (RMT) code[3]. RMT is the leading method for describing the multielectron response of atoms to laser light, and we have recently extended its capability to describe molecular systems[4].

The goal of this project is to extend our knowledge of ultrafast electron dynamics into molecular systems, by performing some of the first calculations for molecules in strong fields with RMT. This will require a detailed exploration not only of the physical parameter space (laser wavelength/intensity, choice of molecule etc.) but also of the limitations of the theoretical approach. Because these simulations will be among the largest ever attempted in this field (employing several tens of thousands of computer cores in parallel), we develop an understanding of how the calculations are best deployed on various supercomputer facilities and may need to introduce new approximation techniques within the codes to make the calculations possible.

Phenomena of current interest include strong field ionisation, photoelectron circular dichroism (probing molecular chirality with chiral light) and photoionisation time delays (time-resolved measurements of electrons escaping atoms and molecules).

The project will leverage our existing partnerships with theorists at the Open University, Charles University, Prague and the University of Colorado, Denver and with experimentalists at the East China Normal University, Shanghai and The Max Planck Institute for Nuclear Physics, Heidelberg. It is expected that you will have the opportunity to visit these and other potential, partners.

Skills gained by student

This project will put you at the forefront of computational physics and will teach you skills of Research Software Engineering and high-performance computing, as well as the more specialised techniques within atomic and molecular physics.

Useful references

1. The Nobel Prize in Physics, 2023
2. Calegari *et al.* J Phys. B. **49** 062001 (2016)
3. Brown *et al.* Comput. Phys. Commun. 250 107062 (2020)
4. Benda *et al*. Phys. Rev. A 102 052826 (2020)