Project title: Ultra-fast atomic dynamics in X-ray FEL light

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Helpful existing knowledge:	Quantum Mechanics (such as MTH4031, MTH3032, PHY3001)
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Project Description:

This project investigates the application of computational techniques for the description of ultra-fast atomic processes to atoms in state-of-the-art free-electron laser light. As explained in the scientific background to the 2023 Nobel Prize for Physics [1], high-harmonic generation has allowed experiment to observe the motion of electrons inside an atom. Techniques [2] developed at Queen's can provide computational evidence that such experiments are indeed giving the correct answers (see eg [3]). So far, this correspondence has been demonstrated for outer electrons, but in this project, we want to apply our techniques to study the role of inner-shell electrons.

Inner-shell electrons are bound more tightly to the nucleus than outer-shell electrons. New light techniques are thus needed to investigate their dynamics. Numerous countries have constructed free-electron laser facilities for the generation of exactly this type of light. This energetic light creates new dynamics, but as both outer and inner electrons can respond simultaneously, the experimental observations are difficult to understand. Therefore, major theoretical and computational efforts are urgently required.

In this project, we will investigate ultra-fast atomic processes initiated by X-ray laser light of relevance to experiment. Initially, we will focus on X-ray initiated Raman spectroscopy [4]. This process could be applied to generate proper laser pulses from X-ray FEL laser light. The original FEL laser light is incoherent, but stimulated Raman emission could yield coherent laser light. The main idea is to create a population inversion by excitation of a 1s electron in neon (in the $1s^2 2s^2 2p^6$ ground state) to the open 3p shell. This creates a population inversion for the 2p electrons, which now see a vacancy in the 1s shell. This opens the possibility of generating proper XUV laser light. We will explore the atomic physics of this process first of all, whereas later studies may focus on the dynamics of ionized Ne^+ ions with a core vacancy.

Useful references

[1] Advanced information. NobelPrize.org. Nobel Prize Outreach 2025. Tue. 28 Oct 2025. <https://www.nobelprize.org/prizes/physics/2023/advanced-information/>

[2] A.C. Brown *et al*, Computer Physics Communications **250**, 107062 (2020)

[3] W. Jiang *et al*, Nature Communications **13**, 5072 (2022)

[4] A.S. Morillo-Candas *et al*, arXiv:2408.11881 (2024)