Ph.D. Project 2022

Photoionization Cross Sections for Astrophysically Important High Z Species

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Background and Motivations

Nearly all modern observational research in gaseous nebulae, whether ground or satellite based, involves a spectra whose interpretation requires an understanding of the atomic processes involved and the handling of atomic data. Numerous atomic datasets are required to model these observations – data such as electron-impact excitation rates, oscillator strengths, transition probabilities and photoionisation cross sections. The demands on the quality and quantity of the atomic data provided has grown dramatically with the advent of new satellite and ground based programmes, which deliver observational data with far greater spectral resolution and sensitivity than ever before. It is therefore imperative that all atomic data evaluated is of the highest accuracy.

For the astrophysically important ions of interest in this project difficulties arise because of the presence of an open 3d-shell in the description of the target ion, which gives rise to hundreds of target state energy levels and typically thousands of closely coupled channels. To overcome these difficulties new and pioneering R-matrix codes have been developed which are capable of exploiting national and international HPC facilities, and which now make the above calculations computationally feasible. A huge amount of work has already been carried out by our group in the ARC research division. Structure models have been developed for the following Fe-peak ions Sc II, Ti II, Cr II, Mn II, Fe II, Fe III, Ni II, Ni III, and Ni V, and these models have been incorporated into scattering calculations to evaluate collision strengths and effective collision strengths for use in astrophysical applications. The associated photoionisation cross sections are also required for these ions to model photoionised plasmas and this work forms the workload of the current PhD proposal.

The ejection of an electron by an atom or ion following the absorption of a photon is described as photoionisation and the process can be typically described by the following equation

$$A + h\nu \longrightarrow A^{+} + e^{-}$$

Where the final state A^{+} is referred to as the N-electron target and the initial state A is a bound state of the composite $(N+1)$-system. Within the R-matrix framework, therefore, photoionisation of ion A^{n+} is closely related to the electron scattering of ion $A^{(n+1)+}$ and hence we may use the same target state wavefunctions as input into the calculation. All the target models we have created for the scattering calculations may be adopted again for use in the photoionisation work. This will allow us to provide a complete and consistent of atomic data for each ion for use in astrophysical applications and modelling. **Objectives & Methodology**

- To compile and test the latest R-matrix photoionisation codes on our local machines or alternatively on the national and international HPC computer facilities.
- To use some of the models already established for the Fe-peak ions and evaluate both ground and excited state photoionisation cross sections.
- To incorporate the complete and consistent set of atomic data for each ion considered into the CLOUDY modelling codes to perform diagnostic applications. This collaboration is alongside our colleagues in the University of Kentucky and Auburn University.
- To incorporate the photoionisation cross sections for the ground and excited states of each ion into the opacity modelling codes in collaboration with the group at the Observatoire de Paris.

Required skills

- Previous experience with programming would be beneficial. A large component of the project shall be computational , and an interest in developing these skills on local parallel computing platforms and/or national/international supercomputers is required.
- A basic understanding of introductory quantum mechanics and atomic structure would also be beneficial.
- An interest in astrophysics and modelling.

Further information

For further information, please contact c.ramsbottom@qub.ac.uk or c.ballance@qub.ac.uk.