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

Ph.D. Project 2019-2021

Propagating Uncertainty in R-matrix calculations through to plasma diagnostics

Project supervisors: **Dr Connor Ballance and Dr Catherine Ramsbottom**
Contacts: **c.ballance@qub.ac.uk**

State of the art and motivations

Newly developed relativistic R-matrix codes that harness the capabilities of Europe's supercomputer network have been developed at QUB. They are the foundations of both the time-independent and laser-atom time-dependent codes within CTAMOP. It allows us to take accurate description of atomic (and molecular) targets from first principle structure and subject them to electron/photon/multi-photon bombardment. However as well as fundamental collision theory, the work has direct application within magnetically-confined and astrophysical plasmas.

Objectives & Methodology

The success in carrying-out accurate R-matrix calculations for processes such as electron-impact excitation, ionisation, recombination and photoionisation in a reasonable time has allowed us to return to the question of uncertainty on such results. Experimentalists for decades have asked for an uncertainty on theoretical simulations analogous to errors on experimental measurement. Plasmas diagnostics are constructed from various collisional processes as well as local plasma conditions. However, we propose taking each of these processes, and through a Monte-Carlo method propagate the correlated uncertainty associated with each process through to the diagnostic. This process of associating uncertainty within new calculations is now a formal requirement of publishing in journals such as Physical Review A or J Phys B.

For example if we take photoionisation as a test case: As stated in Sterling *et al* 2015, the "abundance determinations of Se and Kr and indeed all n-capture elements in astrophysical nebulae are plagued by uncertainties. The most important of these uncertainties stems from the absence of reliable atomic data. However, atomic data needed to reliably correct for the abundances of unobserved ionization stages are unknown." Such "ionization correction factors," or ICFs, are most reliably derived via numerical simulations of astrophysical nebulae (Kingsburgh Barlow 1994; Kwitter Henry 2001; Rodreguez Rubin 2005; Delgado-Inglada et al.2014 (see references with Sterling paper). However, the simulations are only as accurate as the underlying atomic physics that they include.

Collaborations

On the magnetic fusion side we pursue these ideas with the group at Auburn University who have several large scale fusion devices as well as a strong collaboration with an industrial scale device called D-III-D at General Atomics, Ca. On the astrophysics side, as well as strong local collaborations with Dr Stuart Sim (ARC) we collaborate with Prof Phillip Stancil (University of Georgia), and Drs Jim Babb and Adam Foster (Harvard Smithsonian Center for Astrophysics). For the stellar opacity work, Dr Franck Delahaye is our point of contact at the Observatoire de Paris, who accepts our photoionisation calculations for his opacity codes.

Required skills

It would be beneficial if the prospective student has an entry-level quantum mechanical course. There is the intent that the student would develop, calculate and employ the resulting fundamental atomic data with numerical simulations. Therefore, an interest in solving problems from first principles and an interest in programming on large scale parallel computer architectures with the end focus of applying these results to the interpretation of astrophysical observation is important. However, more important is an interest in the topic as these skill-sets can be acquired during the project.

Further information

Contact either Dr Connor Ballance (c.ballance@qub.ac.uk) or Dr Catherine Ramsbottom (c.ramsbottom@qub.ac.uk)

References

[1] N Sterling *et al* ArXiv:1505.01162v1 [astro-ph.SR] 5 May 2015