Centre for Theoretical Atomic, Molecular, and Optical Physics

Ph.D. Project 2021-2024

Relativistic R-Matrix Calculations in the EUV/soft X-ray energy regime

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Motivations

Cosmic x-ray and EUV spectroscopy has entered a Golden Era, with a wide range of high-resolution spectrometers observing the Sun, the solar system, and distant astrophysical sources as well as new facilities in development for launch [1]. Placing the spectrometer beyond the Earths atmosphere, each mission represents a major investment by NASA, ESA, or JAXA, typically requiring at least an order of magnitude improvement over previous mission. Upcoming missions, such as XRism or Athena, will further push bandpass accuracy down to $0.1 - 6.2$ nm which demands a similar upgrade in the theoretical calculations that underpin the interpretation of this observed spectra.

Objectives & Methodology

Within the collision group of CTAMOP, we develop relativistic scattering and photoionisation codes that need theoretical refinement if we are to address these problems. The R-matrix method, DARC (Dirac Atomic R-matrix Codes) although already a level-resolved scattering code, does not fully account for the relativistic properties of the incident electron if its energy exceeds 1000-1500 Rydbergs i.e.a significant fraction of the speed of light. Therefore, this project would involve an extension of both the theory and its implementation within the current suite of codes, by solving equations of the form

$$(\frac{\mathrm{d}}{\mathrm{dr}} + \frac{\kappa_i}{r})P_{ij}^{J\Pi}(r) - \frac{1}{c}(2c^2 + \epsilon_i + \frac{z}{r})Q_{ij}^{J\Pi}(r) = -\frac{1}{c}\sum_{i'=1}^{n} V_{ii'}^{J\Pi}(r)Q_{i'j}^{J\Pi}(r) \quad i = 1, \ldots, n$$

$$(\frac{\mathrm{d}}{\mathrm{dr}} - \frac{\kappa_i}{r})Q_{ij}^{J\Pi}(r) + \frac{1}{c}(\epsilon_i + \frac{z}{r})P_{ij}^{J\Pi}(r) = \frac{1}{c}\sum_{i'=1}^{n} V_{ii'}^{J\Pi}(r)P_{i'j}^{J\Pi}(r) \quad i = 1, \ldots, n$$

where P and Q are continuum radial orbitals, κ_i the angular momentum of the incident electron, ϵ_i relates the channel energies, and $V_{ii'}$ a potential matrix coupling channels together[2].

Collaborations

These developments align well with the goals our colleagues from ARC, whose kilanova simulations under certain conditions may benefit from the inclusion of higher order relativistic cross sections and rates.

We also have ongoing collaborations locally, with Prof. Simon Jeffries at Armagh Planetarium(N.I), with Dr Franck Delahaye at the Observatoire de Paris (EU) concerning stellar opacities, as well as colleagues at Auburn University (US) and the Harvard Centre for Astrophysics (US) where they build and develop spectrometers.

Required skills

- At least an introductory course in Quantum Mechanics.
- Taking the lead in implementing these additions to the existing code-base.
- An interest in High Performance Computing as these simulations will require the use of our parallelized suite of codes
- An interest in visiting other institutions for short periods of time, as well as presenting your work at conferences and workshops.

Further information

Email: c.ballance@qub.ac.uk, if you have further questions or require more details.

References

[1] Randall Smith it et al J. Phys. B: At Mol Opt. Phys **53** 092001 (2020).

[2] 'R-matrix Theory of Atomic Collisions', Phillip Burke, Springer Publishing, ISBN 978-3-642-15930-5, pp.284-285 (2011)