Project title: A Dirac R-matrix approach to the determination of opacities.

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Helpful existing knowledge: Numerical analysis , intro quantum module

Funding status: None

Closing date: As prescribed by website

Overview

Opacities are key ingredients in any domain where radiative transfer is important. In particular, Rosseland mean opacities play an essential role in stellar modelling. They characterize the interaction between the photons produced in the center of stars and the surrounding plasma up to the surface of the stars. Bound-Bound (atomic structure) transitions and bound-free(photoionisation) transitions underpin the accurate determination of such opacities, which our atomic collision group are able to calculate quite accurately.

For the stellar opacities, until 2015, there was essentially agreement between all of the theoretical opacity models, however a Sandia experiment challenged that idea. The measurement at Sandia National Laboratory of the Fe opacity at 180 eV and Ne = 3.1x10^{22} cm^{-3} , which is in line with conditions corresponding to the base of the Solar convection zone:**Te** 2.15 x 10^6 K and **Ne** 3.1 x 10^{22} cm^{-3}$ measured an opacity of a factor of 2 higher than all calculations and exhibits large differences at certain photon energies (Bailey et al. 2015; Nagayama et al.2019). We shall investigate Fe as well as two other Fe-peak elements Cr and Ni.

Plan of work

The project shall proceed as follows. There shall be a review of the underlying Dirac R-matrix approach to photoionisation and di-electronic recombination as well as the equivalent perturbative approaches as implemented within the code AUTOSTRUCTURE. The student will familiarize themselves with theory as implemented within a large suite of parallel codes.

The student will be responsible for carrying out the majority of the Cr and Ni photoionisation calculations for Fe-peak elements. This involves the Na to O-like ion stages for each of these five elements.

Background

It would be beneficial if the prospective student has had an entry-level quantum mechanical course. There is the intent that
the student would develop , with guidance, their own photoionisation models. Therefore, some basic understanding of numerical methods with either Python, Matlab, C++ , Fortran or their more modern equivalents would

be desirable. However, more important is an interest in the topic as these skill-sets can be acquired during the project

Contact

If you have any questions, do not hesitate to send an email to: c.ballance@qub.ac.uk

References

Bailey J. E. et al., 2015, Nature, 517, 56
Nagayama T. et al., 2019, Phys. Rev. Lett., 122, 235001