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

Ph.D. Project 2020-2023

Relativistic Dirac R-matrix photoionisation calculations through to their implementation with stellar opacity codes

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State of the art and motivations

Stellar [1] opacities are underpinned by the accuracy of many atomic structures and how we model the interaction of photons with them. At QUB we have developed a suite of parallel R-matrix codes to calculate the photoabsorption/photoexcitation most astrophysically relevant elements of the periodic table. For elements $\leq Z = 30$ we have a semi-relativistic Breit-Pauli code, and a fully relativistic Dirac code for anything else. We are in the unique position at QUB to start from first principles at the atomic structure level, carry-out the bound-bound (atomic structure), bound-free (photoionisation/photoabsorption) and the free-free transitions that are the constituent parts of an opacity and assess their impact.

Objectives & Methodology

Opacities are usually a mixture of several species, and different ion stages, but we shall initially focus of Fe-peak elements from Cr-Ni. Your goal will be to calculate the photoabsorption cross section these elements, from 16^{+} to 19^{+} and to insert these elements within our opacity code to assess their impact [2]. To carry out these calculations within a finite period of time, large scale parallel (MPI enabled) R-matrix codes have been developed that now harness the power of Graphical Processor Units (GPUs) as well. Therefore, an interest in programming on a wide range of supercomputers is necessary.

Collaborations

This work is supported under the STFC consolidated grant, therefore heavy atomic systems such as Au and Pt that integrate with the modelling codes of Dr Stuart Sim will take a priority. However, we have long-term collaborations under the International Opacity Project, with close associations with the Dr Franck Delahaye (Observatiore de Paris) and with Prof Nigel Badnell at the University of Strathclyde. There will be opportunities to spend some time at either of these institutions.

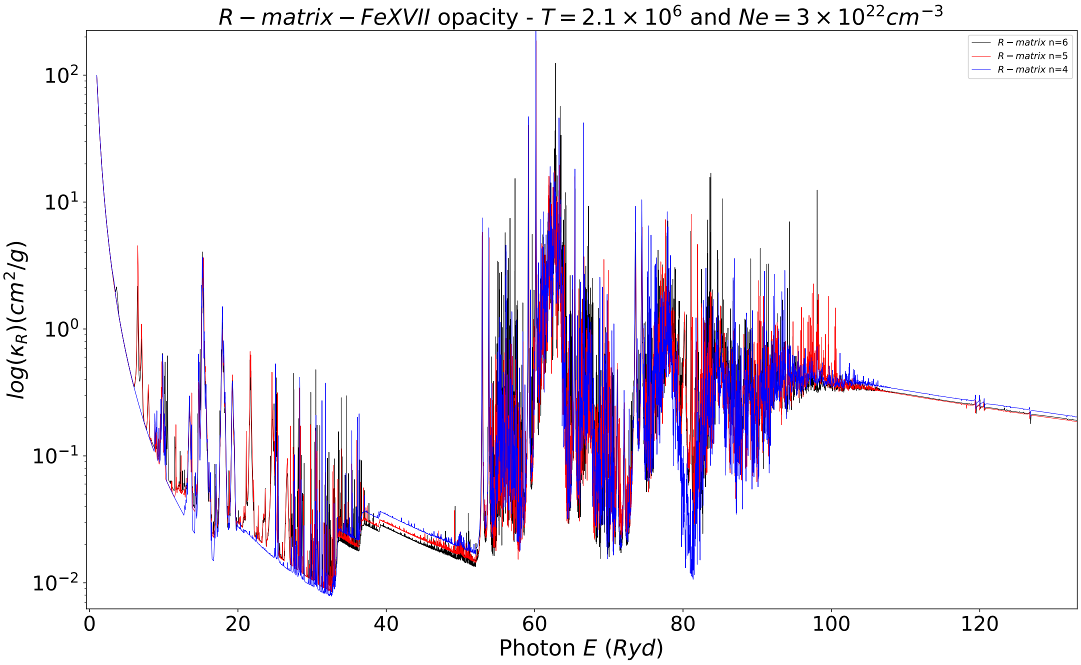

Figure 1: Monochromatic opacities for Fe XVII for R-matrix calulations of different sizes. At the prescribed density and temperature, the $n = 4$ (267 level), $n = 5$ (407 level) and $n = 6$ (640 level) calculations show the slow convergence to completeness. The strength of the R-matrix method is that it includes all resonance structure inherently within it.

Required skills

- An introductory quantum course is preferred, though not required
- An interest in fundamental atomic structure and collisions
- An interest in high performance computing
- To collaborate at different institutions and present work either via talks or poster presentations at International meetings

Further information

Either email: c.ballance@qub.ac.uk or arrange a meeting.

References

[1] Hummer D G and Mihalas D, Ap J 331, 794 , 1988

[2] Seaton M J, MNRAS 289, 700, 1997