T2a

A non-perturbative R-matrix tutorial for single photon ionization of atoms and ions

Connor Ballance[1], **Nigel Badnell**[2], **Franck Delahaye**[3]

[1] *School of Maths and Physics, Queen's University of Belfast, UK*
[2] *Department of Physics, Strathclyde University, UK*
[3] *LERMA, Observatoire de Paris; PSL Research University; CNRS; Sorbonne University, France*

This joint lecture will present two generalized approaches for calculating the cross sections of fundamental atomic processes, with an emphasis on the single photon ionization of atoms and ions. The distorted-wave method is categorized as a perturbative approach and shall be presented by Dr Fontes, whereas the R-matrix method, which is a non-perturbative method will be presented by myself.

A summary overview of the R-matrix method and associated terminology given in greater detail in the R-matrix review book of P. G. Burke [1] shall be given. A discussion concerning the strengths and weaknesses of the method, sometimes in relation to the distorted-wave method will be provided highlighting the computational bottlenecks and how we address them. These include the description of Rydberg resonance structure in the two methods and how we optimize the structure for photo-ionization calculations.

A simple He-like Fe test case for those attendees that would like to pursue a calculation themselves and the step-by-step process from atomic structure to photo-ionization cross sections will be presented.

For the vast majority of highly charged ions there is wide applicability of both distorted-wave and R-matrix methods and excellent agreement found between them in terms of the fundamental photo-ionization cross sections. In terms of application, the R-matrix approach provides the bound-bound and bound-free component of opacity calculations [2] for many ion stages. Opacities shall be discussed in greater detail by Dr Fontes.

Further Reading

1. P. G. Burke, "R-Matrix Theory of Atomic Collisions", Springer (2011); doi:10.1007/978-3-642-15931-2.
2. F. Delahaye, C. P. Ballance, R. Smyth and N. R. Badnell, "Quantitative comparison of opacities calculated using the R-matrix and Distorted-Wave methods: Fe XVII", *Monthly Notices of the Royal Astronomical Society* **508**, 421 (2021); doi:10.1093/mnras/stab2016.

Presenting Author Email Address: *C.Ballance@qub.ac.uk*