# Atomic cross section calculations: the distorted-wave method

**Christopher J. Fontes**[1]

[1]*Computational Physics Division, Los Alamos National Laboratory, USA*

Over the past sixty years, steady and significant progress has been made in the ability to calculate the vast amount of atomic data that is required to model spectra produced by plasmas, under both local thermodynamic equilibrium (LTE) and non-LTE conditions. Ab initio methods for calculating the cross sections associated with fundamental atomic processes typically fall under two categories: close-coupling theory and distorted-wave theory. The former is sometimes referred to as a "non-perturbative" approach, in which the continuum and bound electrons are treated on an equal footing, and are coupled (or mixed) in a single wavefunction. The latter is considered to be a perturbative approach, in which the continuum-electron wavefunctions are calculated in the presence of a distortion potential that is produced by previously calculated bound-electron wavefunctions. In this case, the continuum and bound electrons are not formally mixed.

This presentation is the second half of a joint talk given by Dr. Ballance, who will discuss the non-perturbative R-matrix method, and myself. The goal of this talk is to provide a basic explanation of the distorted-wave method, particularly in the context of so-called "resonances" that can appear in the atomic cross sections. Resonances may occur when a continuum electron appears in a fundamental atomic process, either at the start or the end of the process, and at least two bound electrons are present in the target atom or ion. More specifically, resonances can appear in the cross sections associated with the processes of electron-impact excitation, electron-impact ionization and photoionization, as well as their inverse processes. In the distorted-wave approach, the resonance contribution can be calculated via a two-step process that begins with a specific bound state, followed by a short-lived autoionizing state that spontaneously decays (via the Auger-Meitner process) to a specific final bound state of interest. The calculation of resonances via this two-state approach was pioneered, for the process of dielectronic recombination, by Bates and Dalgarno [1] and subsequently applied in the analysis of solar spectral features by Gabriel, Jordan and Paget [2,3], while the process of electron-impact excitation was investigated by Seaton [4] and Cowan [5].

In this talk, I focus on the process of photoionization, which is important from both a fundamental-theory perspective and the practical need to provide the so-called "bound-free" contribution to the radiative opacity, which

is important for an understanding of stellar structure. I use the Los Alamos Suite of Atomic Physics Codes [6] to calculate photoionization cross sections for some simple examples and demonstrate, for highly charged ions, that the resulting cross sections produce very similar results to those obtained with the R-matrix solution to the close-coupling equations.

## Further Reading

1. D.R. Bates and A. Dalgarno, in *Atomic and Molecular Processes*, Ed. D.R. Bates (New York: Academic) pp. 258–61 (1962).

2. A.H. Gabriel and C. Jordan, Nature **221**, 941 (1969).

3. A.H. Gabriel and T.M. Paget, J. Phys. B: Atom. Molec. Phys. **5**, 673 (1972).

4. M.J. Seaton, J. Phys. B: Atom. Molec. Phys. **2**, 5 (1969).

5. R.D. Cowan, J. Phys. B: Atom. Molec. Phys. **13**, 1471 (1980).

6. C.J. Fontes, H.L. Zhang, J. Abdallah, Jr., R.E.H. Clark, D.P. Kilcrease, J. Colgan, R.T. Cunningham, P. Hakel, N.H. Magee and M.E. Sherrill, J. Phys. B **48**, 144014 (2015).

## Acknowledgements

Presenting Author Email Address: *cjf@lanl.gov*