Atomic Data Needs for X-ray Astronomy. 22 June 2000
http://heasarc.gsfc.nasa.gov/docs/heasarc/atomic/
M. A. Bautista, T. R. Kallman, and A. K. Pradhan, eds.

The R-matrix with Pseudostates Method

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Abstract. We review the development of pseudostate methods for treating electron-ion collision processes. We describe our implementation of these methods within the Wigner–Eisenbud R-matrix method. We present recent results for photoionization, electron-impact excitation, and electron-impact ionization, which demonstrate the importance of properly accounting for the two-electron continuum. The comparison with experimental, as well as other theoretical, electron-impact ionization results suggests that there may be inaccuracies in the overall normalization of earlier measurements. This is confirmed in the case of Al^{2+} by a more recent experimental study. The implications regarding the use of excitation and ionization rates from existing databases for modeling astrophysical plasmas are discussed.

1. Introduction

The close-coupling method (Massey and Mohr 1932), as developed for continuum Hartree-Fock solutions by Seaton (1953), has proven to be a practical means for studying electron–ion collision phenomena because the individual behavior of both the colliding and ionic electrons is revealed. In its most general form, the close-coupling wavefunction for a quasi two-electron system can be expanded as the sum of product wavefunctions (angular coupling and antisymmetrization are assumed):

$$\Psi(\vec{r_1}, \vec{r_2}) = \sum_i \Phi_i(\vec{r_1}) f_i(\vec{r_2}) + \int d\vec{k} \Phi_{\vec{k}}(\vec{r_1}) f_{\vec{k}}(\vec{r_2}) \ . \tag{1}$$

In this close-coupling expansion, Φ_i and $\Phi_{\vec{k}}$ are the (denumerably infinite) bound and (indenumerably infinite) continuum wavefunctions of the one-electron ion, and f_i and $f_{\vec{k}}$ are the wavefunctions for the scattering electron, which are determined by solving the close-coupling equations. The R-matrix method (Burke and Berrington 1993), in particular, is widely used for this purpose.

Of course, only a finite close-coupling expansion can be used in any numerical treatment. It is the choice of which terms to retain that truly defines the art of performing electron-ion collision calculations within basis expansion methods. The earliest close-coupling calculations for electron-hydrogen collisions could only include the lowest six states $(1s, 2s, 2p, 3s, 3p, 3d)$, given the computational power available at the time. However, it was pointed out by Castillejo et al. (1960) that the atomic polarizability, which is given by

$$\alpha = \sum_{\substack{n>1 \\ \ell}} \frac{\langle \Phi_{1s}|\vec{r}|\Phi_{n\ell}\rangle\langle \Phi_{n\ell}|\vec{r}|\Phi_{1s}\rangle}{E_{n\ell} - E_{1s}} + \sum_{\ell} \int dk \frac{\langle \Phi_{1s}|\vec{r}|\Phi_{k\ell}\rangle\langle \Phi_{k\ell}|\vec{r}|\Phi_{1s}\rangle}{E_{k\ell} - E_{1s}}, \tag{2}$$

received an 18.4% contribution from the second term in Equation (2). This means that the two-electron continuum must be included in order to accurately describe the polarization of the hydrogen atom by an incoming electron. Indeed, the seminal close-coupling calculations on e^-–H by Burke et al. (1963) found a major disagreement with experimental results for the 1s → 2p excitation. Burke and coworkers had truncated their atomic expansion to the $n = 3$ states and they concluded that "these discrepancies probably can not be reconciled by any close-coupling expansion", referring to the denumerably infinite number of bound terms Φ_i in Equation (1).

In subsequent studies, and following the Sturmian basis set ideas of Rotenburg (1962), Burke et al. (1969) introduced into the close-coupling expansion the so-called *pseudostates.* These are unphysical orbitals which in general overlap with both the bound and continuum hydrogenic orbitals $\Phi_{n\ell}$ and $\Phi_{k\ell}$. A distinctly improved convergence over the earlier e^-−H results was obtained but non-trivial discrepancies with experiment remained. Despite remarkable advances in computational power over the next two decades, and the development of more sophisticated pseudostate methods (e.g. Scott et al. 1989, and reference therein) the disagreement between theory and experiment for e^-−H collisions remained unresolved.

Then, in 1992, Bray and Stelbovics (1992) resolved the discrepancy by performing *Converged Close-Coupling* (CCC) calculations. They solved the Lippmann-Schwinger (momentum-space) equations with a large expansion of Laguerre pseudoorbitals and obtained e^-−H elastic and excitation cross sections that were in good agreement with experiment. This was an important triumph for it indicated that the indenumerably infinite two-electron continuum expansion in Equation (1) could be adequately represented by a finite pseudostate expansion. Furthermore, it was found that electron-impact ionization cross sections could be extracted by analyzing the excitation to pseudostates Bray and Stelbovics (1993).

Following up on this encouraging breakthrough, Meyer and Greene (1994) applied a large pseudostate expansion within their (position-space) Eigenchannel R-matrix method and were able to calculate helium photo-double-ionization cross sections in excellent agreement with the latest experimental results (Meyer et al. 1997). This achievement was particularly important because it demonstrated that the R-matrix method could be used to perform converged pseudostate calculations, at least in principle.

The Belfast (Wigner-Eisenbud) R-matrix codes (Burke and Berrington 1993; Berrington 1995) are extremely robust in that they can be used to study electron-ion systems of arbitrary complexity. Having found essentially equivalent results using two separate R-matrix codes in a joint study (Bartschat and Green 1993) the success of the Eigenchannel R-matrix method for treating the two-electron continuum suggested that the Wigner-Eisenbud R-matrix method should be capable of the same. Indeed, after overcoming some tricky issues dealing with non-orthogonal orbitals and unphysical R-matrix poles, Bartschat et al. (1996) developed the *R-matrix with Pseudostates* (RMPS) method for use within the Belfast R-matrix codes. Bartschat and coworkers have successfully applied their RMPS method to treat two-electron processes in the photoionization and electron-impact excitation and ionization of numerous atomic systems (Bartschat 1998).

2. Two-Electron Photoionization Processes

The present implementation of the RMPS method (Gorczyca and Badnell 1997) arose independently from that of Bartschat and coworkers in response to a void of theoretical calculations for the higher-n photoionization-excitation of helium:

$$h\nu + \mathrm{He}(1\mathrm{s}^2) \rightarrow \mathrm{He}^+(n\ell) + e^- \ . \tag{3}$$

In particular, the effective angular distribution parameter β^{eff}, which characterizes the differential photoionization-excitation cross section via

$$\frac{d\sigma_{n\ell}}{d\Omega} = \frac{\sigma_{n\ell}}{4\pi}\left[1 + \beta_{n\ell}P_2(\cos\theta)\right] \ , \ \text{and} \ \beta_n^{eff} = \frac{\sum_{\ell=0}^{n-1}\sigma_{n\ell}\beta_{n\ell}}{\sum_{\ell=0}^{n-1}\sigma_{n\ell}} \ , \tag{4}$$

had been measured for $n = 2-6$, yet theoretical calculations only existed for $n = 2$ (Wehlitz et al. 1993). It was immediately found that a standard R-matrix approach for treating the $n = 3$ processes which used only physical orbitals (basis set 1) showed major qualitative differences from the observed behavior (see Figure 1), especially on using the length form of the dipole operator (this places more emphasis on the large-r portion of the wavefunction). Whereas the angular distribution should have the high-energy behavior $\frac{d\sigma_3}{d\Omega} \approx \cos^2\theta$ ($\beta \rightarrow 2$) due to the dominance of the 3s excitation, the length form using basis 1 shows a nearly isotropic result ($\beta \approx 0$) at 200 eV. The use of physical states alone seriously fails to describe even the qualitative nature of the ionized electron's angular distribution.

On first introducing pseudoorbitals into the close-coupling expansion, we encountered severe difficulties with regards to the issues of the non-orthogonality of basis functions and unphysical R-matrix

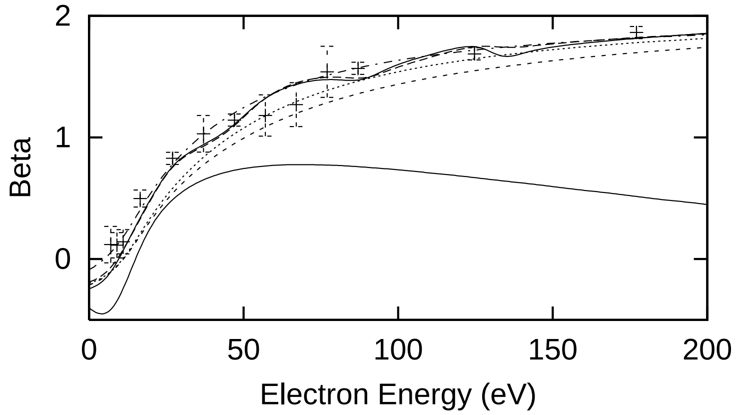

Figure 1. RMPS asymmetry parameters for $h\nu + \mathrm{He}(1s^2) \rightarrow \mathrm{He}^+(3\ell) + e^-$: basis 1, length (full curve) and velocity (chain curve), basis 2, length (dashe d curve) and velocity (broken curve), and basis 3, length (full curve) and velocity (lon gbroken curve) results. The basis 1 length curve invariably shows the poorest overall behavior compared to the others. The experimental values ($\diamond$) are from Wehlitz et al. (1993).

poles. We found it essential to modify the codes in order to 1) implement a stable Gram-Schmidt orthogonalization procedure for overlapping basis sets which retained only the minimum set of linearly independent orbitals, and 2) use a *different* Buttle correction (Burke and Berrington 1993) which takes into account the use of non-orthogonal orbitals (Gorczyca and Badnell 1997). The agreement obtained with experiment is much better on using pseudoorbitals to improve the ground-state wavefunction (basis set 2), but there is still a noticeable split between the length and velocity results. The two are finally brought into close agreement when pseudoorbitals are used to describe the final continuum state as well. We point out that, on using several pseudoorbitals — even in the ground state description alone, the above two modifications were crucial for obtaining meaningful scattering information.

3. Double Continuum Effects in Electron-Impact Excitation

In a recent study (Griffin et al. 2000), the RMPS method was used to study electron-impact excitation in C^{3+} and O^{5+}. A comparison of results from a standard R-matrix calculation and an RMPS one are shown in Figure 2. It is seen immediately that the effect of the double continuum is to cause a reduction, by as much as a factor of two, in the computed cross section over a wide range of energies. Of course, this level of correction due to the double continuum occurs only for excitation to the $n = 4$ states and higher; excitation to the lower terms show smaller effects. Still, this suggests that many electron-impact excitation rates currently in data bases that are used by plasma modelers may be an overestimate since they are normally computed using standard close-coupling (i.e. non-pseudostate) methods.

4. Electron-Impact Ionization

The sum of electron-impact excitation cross sections to pseudostates that lie above the ionization limit can be interpreted as an ionization cross section, since the pseudostates have predominantly continuum character. Together with two completely independent approaches — the well-known *Distorted Wave* (DW) method and the *Time-Dependent Close-Coupling* (TDCC) method — we performed RMPS calculations for three ions of the Li-like sequence, Be^+ (Pindzola et al. 1997), B^{2+} (Woitke et al. 1997; Marchalant et al. 1997), and C^{3+} (Mitnik et al. 1999). We compared our calculated ionization cross sections to existing experimental results — for Be^+ (Falk and Dunn 1983), B^{2+} (Crandall et al. 1986; Experiment (b) in Figure 3), and C^{3+} (Crandall et al. 1982), and a new experimental result for B^{2+} (Woitke et al. 1997) (Experiment (b) in Figure 3). An important trend is highlighted in the figures: (1)

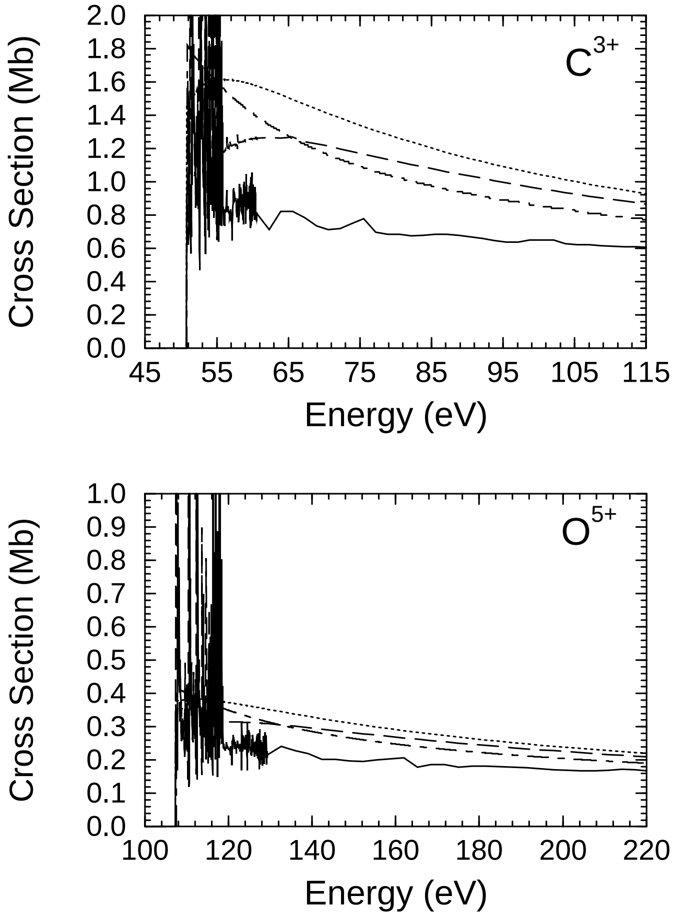

Figure 2. Electron-impact excitation cross sections for the 2s → 4d transition in C^{3+} and O^{5+}. The dotted curves are from a 9-state non-pseudostate R-matrix calculation; the dashed curves are from a 13-state non-pseudostate R-matrix calculation; the solid curves are from a 41-state RMPS calculation; and the dot-dashed curves are from the fitting formula of Fischer et al. (1997).

the experimental results are much larger than the theoretical ones for Be^{+}; (2) the experimental and theoretical results are about the same for B^{2+}; (3) the experimental results are significantly less than the theoretical results for C^{3+}.

The excellent agreement between the RMPS and TDCC results tends to suggest that the disagreement with experiment is due to an uncertainty in the normalization of the experiment. This is supported somewhat by the improved agreement between theory and experiment found in the more recent measurements (Woitke et al. 1997; Marchalant et al. 1997), but even more so from a comparison between theoretical and experimental results in another system. In a joint study that used the RMPS, TDCC, and CCC methods to compute the electron-impact ionization cross section of Al^{2+} (Badnell et al. 1998), it was found that, whereas all three *completely independent* theoretical methods gave results in excellent agreement with each other, they were all much larger than the experimental results that existed at that time (Crandall et al. 1998; see Figure 4). As a result of these findings, a new measurement was performed (Thomason and Peart 1998) which gave a cross section that is in much better agreement with the theoretical results, as seen in Figure 4. This is a particularly important example where the theoretical electron-ion studies were able to detect a probable error in the experimental normalization.

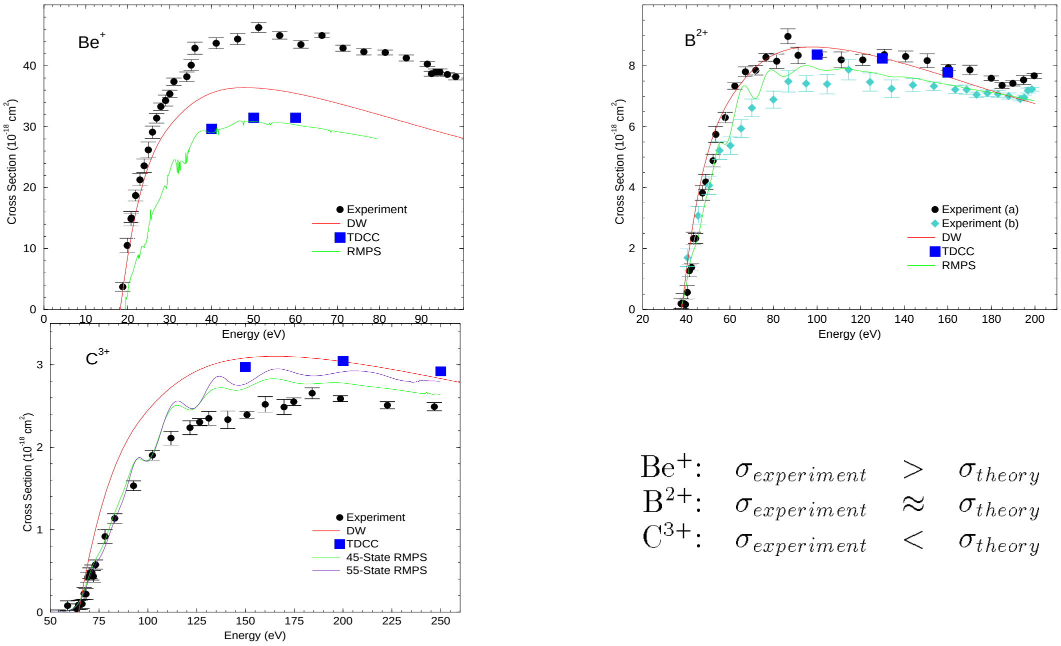

Figure 3. Electron-impact ionization of Li-like ions: comparison between theoretical and experimental results.

5. Conclusion

We have presented a brief review of the history leading up to recent pseudostate work in order to highlight the main ideas behind the RMPS method, and to elucidate the importance of double continuum processes in electron-ion collisions. It has been demonstrated that the use of pseudoorbitals is necessary even just to reproduce the gross features of photoionization angular distributions involving two

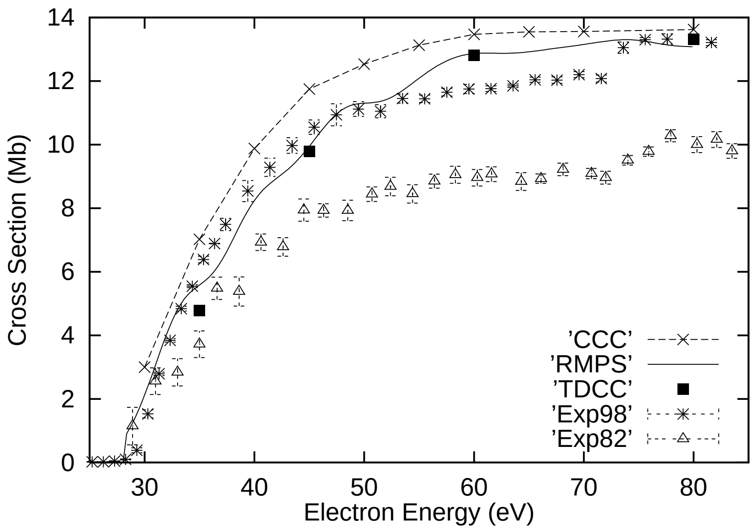

Figure 4. Electron-impact ionization of Al^{2+}: comparison of various theoretical (Badnell et al. 1998), earlier experimental (Crandall et al. 1982) and more recent experimental (Thomason and Peart 1998) results.

electrons. The two-electron continuum was also shown to play an important role in electron-impact excitation, significantly reducing the cross section (by as much as a factor of two) over a wide range of energies. Furthermore, electron-impact ionization cross sections can be extracted from pseudostate calculations. Of particular importance, the results from the RMPS calculations and two other independent state-of-the-art calculations, which are all in excellent agreement with each other, have shown large differences when compared to experimental results, suggesting that the experimental normalization may be incorrect. Indeed, a more recent experimental study in Al^{2+} reported absolute ionization cross sections that are in good agreement with the latest theoretical calculations, and which are much larger than the results of earlier measurements. These findings have important implications for the modelers of astrophysical plasmas since they indicate that many of the atomic rates that exist in databases at present are subject to larger uncertainties than may have been realized in the past.

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