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Atomic Collision Processes for Astrophysical and Laboratory Plasmas

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Abstract. An accurate knowledge of atomic collision processes is important for a better understanding of many astrophysical and laboratory plasmas. Collision databases which contain electron-impact excitation, ionization, and recombination cross sections and temperature dependent rate coefficients have been constructed using perturbative distorted-wave methods and non-perturbative R-matrix pseudo-states and time-dependent close-coupling methods. We present recent atomic collision results.

1. Introduction

Accurate atomic and molecular databases underpin current research efforts in a variety of scientific and engineering areas: including controlled fusion energy, astrophysics, radiation biophysics, fluorescent lamps, and atmospheric pollutant removal. For example, all light elements (H-O) are of interest for fusion experiments; in particular Li and B as wall coating materials and Be and C as primary wall materials.

Over the years both theory and experiment have provided increasingly more accurate cross sections for the electron-impact excitation, ionization, and recombination of atoms and their ions. In this paper we review perturbative distorted-wave methods and non-perturbative R-matrix with pseudo-states and time-dependent close-coupling methods in both their non-relativistic and fully-relativistic versions.

The rest of the review paper is structured as follows: in Section II we describe distorted-wave, R-matrix, and time-dependent close-coupling methods and give an electron-impact ionization cross section example, and in Section III we give a brief review of current projects.

2. Basic Collision Theory

2.1. Configuration-Average Distorted-Wave (CADW) Method

For ionization a general transition between configurations has the form:

$$(n_0 l_0)^{w_0} k_i l_i \rightarrow (n_0 l_0)^{w_0 - 1} k_e l_e k_f l_f \ , \tag{1}$$

where w_0 is a subshell occupation number, $n_0 l_0$ are quantum numbers of the bound electron, and $k_i l_i$, $k_e l_e$, and $k_f l_f$ are quantum numbers of the initial, ejected, and final continuum electrons.

The configuration-average ionization cross section is given by[1]:

$$\sigma_{ion} = \frac{32w_0}{k_i^3}\int_0^{E/2}\frac{d\epsilon_e}{k_e k_f}\sum_{l_i,l_e,l_f}(2l_i+1)(2l_e+1)(2l_f+1)\ \mathcal{S}(n_0l_0k_il_i \rightarrow k_el_ek_fl_f)\ , \tag{2}$$

where $k=\sqrt{2\epsilon}$ and the continuum normalization is one times a sine function.

For excitation a general transition between configurations has the form:

$$(n_1l_1)^{w_1+1}(n_2l_2)^{w_2-1}k_il_i \rightarrow (n_1l_1)^{w_1}(n_2l_2)^{w_2}k_fl_f\ , \tag{3}$$

where w_1 and w_2 are subshell occupation numbers, n_1l_1 and n_2l_2 are quantum numbers of the bound electrons, and k_il_i and k_fl_f are quantum numbers of the initial and final continuum electrons. The configuration-average excitation cross section is given by:

$$\sigma_{exc} = \frac{8\pi}{k_i^3k_f}(w_1+1)(4l_2+3-w_2)\sum_{l_i,l_f}(2l_i+1)(2l_f+1)\ \mathcal{S}(n_1l_1k_il_i \rightarrow n_2l_2k_fl_f)\ . \tag{4}$$

For dense plasmas the initial and final distorted-waves and the Coulomb matrix elements found in $\mathcal{S}(n_0l_0k_il_i \rightarrow k_el_ek_fl_f)$ of Eq.(2) and $\mathcal{S}(n_1l_1k_il_i \rightarrow n_1l_2k_fl_f)$ of Eq.(4) are modified to include an exponential screening factor:

$$SF(r) = e^{-r/\Lambda}\ , \tag{5}$$

where the Debye-Huckel screening radius $\Lambda=\sqrt{T_e/4\pi N_e}$, T_e is the electron temperature, and N_e is the electron density. Fully-relativistic subconfiguration-average distorted-wave ionization and excitation cross sections may also be calculated[2].

2.2. R-Matrix Pseudo-States (RMPS) Method

The R-Matrix method[3] splits the scattering process into two regions. The total wavefunction in the inner region is given by:

$$\Psi_k^{N+1} = \mathcal{A}\sum_{i,j}a_{ijk}\psi_i^{N+1}\frac{u_{ij}(r_{N+1})}{r_{N+1}} + \sum_i b_{ik}\chi_i^{N+1}\ , \tag{6}$$

where $\mathcal{A}$ is an antisymmetrization operator, ψ_i^{N+1} are channel functions obtained by coupling N - electron target states with the angular and spin functions of the scattered electron, $u_{ij}(r)$ are radial continuum basis functions, and χ_i^{N+1} are bound functions which ensure the completeness of the total wavefunction. The coefficients a_{ijk} and b_{ik} are determined by diagonalization of the total $(N+1)$ electron Hamiltonian. The total wavefunction in the outer region is given by:

$$\Psi_k^{N+1} = \sum_i \psi_i^{N+1}\frac{v_i(r_{N+1})}{r_{N+1}}\ , \tag{7}$$

where the radial wavefunctions $v_i(r)$ are obtained by solving the coupled differential equations given by:

$$[T_i(r) + V_{ij}(r)]v_i(r) = 0 \tag{8}$$

where $T_i(r)$ is a kinetic and nuclear energy operator and $V_{ij}(r)$ is an asymptotic coupling operator. The inner and outer region solutions are matched at the boundary and the K-matrix is extracted. Excitation cross sections are obtained by relating the K-matrix to the S-matrix.

Over the years, a non-relativistic RMLS suite of codes has been developed for low Z atoms and ions, a semi-relativistic RMLSJ suite of codes has been developed for medium Z atoms and ions, and a fully-relativistic RMjjJ suite of codes has been developed for high Z atoms and ions. With the addition of pseudo-states, the R-matrix method becomes more accurate for excitation to high-lying excited states. The RMPS method can also be used to calculate electron-impact ionization cross sections, including both direct ionization and excitation-autoionization.

2.3. Time-Dependent Close-Coupling (TDCC) Method

The time-dependent Schrodinger equation for two-active electron atomic systems is given by:

$$i\frac{\partial\Psi(\vec{r}_1,\vec{r}_2,t)}{\partial t} = H(\vec{r}_1,\vec{r}_2)\Psi(\vec{r}_1,\vec{r}_2,t) \ , \tag{9}$$

where

$$H(\vec{r}_1,\vec{r}_2) = -\frac{1}{2}\nabla_1^2 + V(r_1) - \frac{1}{2}\nabla_2^2 + V(r_2) + \frac{1}{|\vec{r}_1-\vec{r}_2|} \ . \tag{10}$$

Expanding in coupled spherical harmonics:

$$\Psi(\vec{r}_1,\vec{r}_2,t) = \sum_{l_1,l_2}\frac{P^{LS}_{l_1l_2}(r_1,r_2,t)}{r_1r_2}\sum_{m_1,m_2}C^{l_1l_2L}_{m_1m_2M}\ Y_{l_1m_1}(\hat{r}_1)\ Y_{l_2m_2}(\hat{r}_2) \tag{11}$$

yields the time-dependent close-coupled equations[4]:

$$i\frac{\partial P^{LS}_{l_1l_2}(r_1,r_2,t)}{\partial t} = [T_{l_1}(r_1)+T_{l_2}(r_2)]\ P^{LS}_{l_1l_2}(r_1,r_2,t) + \sum_{l_1',l_2'}V^{L}_{l_1l_2,l_1'l_2'}(r_1,r_2)\ P^{LS}_{l_1'l_2'}(r_1,r_2,t) \ , \tag{12}$$

where

$$T_l(r) = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{2r^2} + V(r) \tag{13}$$

and $V^{L}_{l_1l_2,l_1'l_2'}(r_1,r_2)$ is a two-body coupling operator.

Fully-relativistic time-dependent close-coupling equations[5] may also be derived based on the time-dependent Dirac equation. After time propagation of the non-relativistic or fully-relativistic TDCC equations, scattering probabilities and cross sections are obtained by projecting the radial wavefunctions onto antisymmetrized products of bound and continuum radial orbitals.

2.4. Comparison of the CADW, RMPS, and TDCC Methods

As an example, we calculated[6] the electron-impact ionization of Al and compared with experiment[7] in Figures 1-2. CADW direct ionization cross sections were included using Eq.(2) for the $3p$ and $3s$ subshells in Figure 1. CADW excitation-autoionization cross sections were included using Eq.(4) for the $3s \rightarrow 3p, 3d$ and $3s \rightarrow 4l(l = 0-3)$ excitations in Figure 1. The CADW total ionization cross section is about a factor of 2 above experiment. TDCC direct ionization cross sections were included for the $3p$ and $3s$ subshells in Figure 2. RMPS total ionization cross sections are also shown in Figure 2. Good agreement is found between the RMPS total ionization calculations and experiment.

2.5. Isonuclear Sequence Databases

Over the last decade light atom isonuclear sequence databases have been assembled based on the most accurate basic collision cross section calculations. Accurate databases are now available for H[8], He[8], Li[9], Be[10], and B[11], while work is in progress for C, N, O, and Ne. Electronic data is available at IAEA/ALADDIN[12]. We also note that previous CADW calculations for the electron-impact ionization of the Fe[13], Ni[14], Kr[15], Sn[16], Xe[16], and W[17] isonuclear sequences are being updated with RMPS and TDCC calculations for the atoms and low-charged ions.

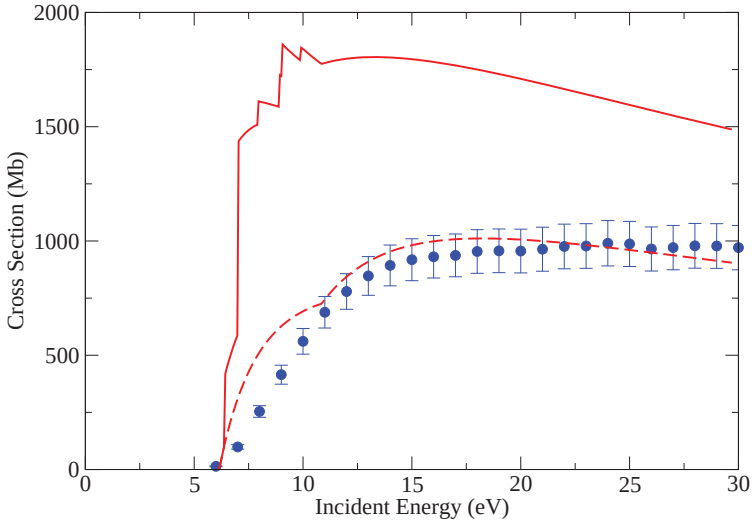

Figure 1. Electron-impact ionization of Aluminum. Solid line (red): CADW total ionization, dashed line (red): CADW direct ionization, circles (blue) with error bars: experiment [7] (1.0 Mb = 1.0×10^{-18} cm^2).

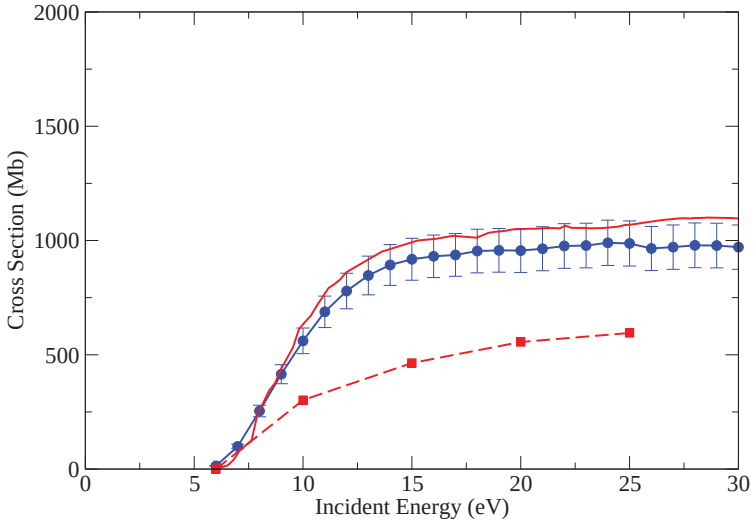

Figure 2. Electron-impact ionization of Aluminum. Solid line (red): RMPS total ionization, dashed line (red): TDCC direct ionization, circles (blue) with error bars: experiment [7] (1.0 Mb = 1.0×10^{-18} cm^2).

3. Summary

We are currently generating accurate electron-impact excitation, ionization, and recombination cross sections for the N isonuclear sequence. In the future we plan to calculate accurate electron-impact excitation and ionization cross sections for atoms and low-charged ions in the Mn, Fe, Co, and Ni isonuclear sequences, as well as in the heavier Mo, Xe, La, W, Au, and U isonuclear sequences.

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