Convergent close-coupling calculation of electron-impact ionisation of H-, He-, Na- and Mg-like ions.

I. Bray, C. Bostock, D. V. Fursa, A. Renwick

Institute of Theoretical Physics, Curtin University of Technology, Perth, Western Australia

4/3/09, IAEA, Vienna
Outline I

1. Introduction
   - Motivation
   - Recent history

2. Nonrelativistic CCC theory
   - atomic target structure
   - electron-atom scattering
   - single and double photoionisation
   - two-centre problems
   - convergence studies

3. Relativistic CCC theory
   - single electron spectrum
   - coupled Lippmann-Schwinger equations
   - Breit and Møller corrections
Outline II

4 Electron-impact ionisation
   - H-like targets
   - He-like targets
   - Na-like targets
   - Mg-like targets

5 Concluding remarks
The primary motivation is to provide accurate atomic collision data for science and industry:

- Astrophysics
- Fusion research
- Lighting industry
- Medical and materials applications

Provide a rigorous foundation for collision theory with long-ranged (Coulomb) potentials, PRL 101 230405 (2008) and Annals of Physics.
Prior to the 1990s theory and experiment generally did not agree for:
- electron-hydrogen excitation or ionisation,
- electron-helium excitation or ionisation,
- single or double photoionisation of helium.

Consequently, we have been developing the convergent close-coupling (CCC) theory for electron/positron/photon/(anti)proton collisions with atoms/ions/molecules that is applicable at all energies for the major excitation and ionisation processes.
Prior to the 1990s theory and experiment generally did not agree for:
- electron-hydrogen excitation or ionisation,
- electron-helium excitation or ionisation,
- single or double photoionisation of helium.

Consequently, we have been developing the convergent close-coupling (CCC) theory for electron/positron/photon/(anti)proton collisions with atoms/ions/molecules that is applicable at all energies for the major excitation and ionisation processes.
Nonrelativistic CCC theory

Structure: using the Laguerre basis $\xi_{nl}(r)$ write:

- "one-electron" (H, Li, . . . , Cs) states:
  $$\phi_{nl}^{(\lambda)}(r) = \sum_{n'} C_{nl}^{n'} \xi_{n'l}^{(\lambda)}(r)$$

- "two-electron" (He, Be, . . . , Hg) states:
  $$\phi_{nls}^{(\lambda)}(r_1, r_2) = \sum_{n', n''} C_{nls}^{n'n''} \xi_{n'l}^{(\lambda)}(r_1) \xi_{n''l}^{(\lambda)}(r_2).$$

Coefficients $C$ are obtained by diagonalising the target (FCHF) Hamiltonian:

$$\langle \phi_f^{(\lambda)} | H_T | \phi_i^{(\lambda)} \rangle = \varepsilon_f^{(\lambda)} \delta_{fi}. \quad (1)$$
Hydrogen $\ell = 0$ energies for $\lambda = 1$ Laguerre bases

Igor Bray <I.Bray@curtin.edu.au>

CCC method for electron-impact ionisation of ions
\[ \phi_{\varepsilon}^{(\lambda)}(r) \] for \( N = 70, \lambda = 2 \) and \( \phi_{\varepsilon}^{(R_0)}(r) \) for \( R_0 = 134 \).
Scattering:

- Electron-atom wavefunction is expanded as

\[
|\psi_i^{(+)}\rangle \approx A \sum_{n=1}^{N} |\phi_n^{(\lambda)}\rangle \langle \phi_n^{(\lambda)} | \psi_i^{(+)}\rangle \equiv A l_N |\psi_i^{(+)}\rangle. \tag{2}
\]

- Solve for \( T_{fi} \equiv \langle k_f \phi_f^{(\lambda)} | V | \psi_i^{(+)}\rangle \) at a total energy \( E \)

\[
\langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle = \langle k_f \phi_f^{(\lambda)} | V | \phi_i^{(\lambda)} k_i \rangle
\]

\[
+ \sum_{n=1}^{N} \int d^3k \frac{\langle k_f \phi_f^{(\lambda)} | V | \phi_n^{(\lambda)} k \rangle \langle k \phi_n^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle}{E + i0 - \varepsilon_n^{(\lambda)} - k^2/2}. \tag{3}
\]

- Have step-function behaviour:

\[
\langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle \approx 0 \text{ for } \varepsilon_f^{(\lambda)} > k_f^2/2.
\]
Scattering:

Electron-atom wavefunction is expanded as

$$\left| \psi_i^{(+)} \right\rangle \approx A \sum_{n=1}^{N} |\phi_n^{(\lambda)}\rangle \langle \phi_n^{(\lambda)} | \psi_i^{(+)} \rangle \equiv A I_N |\psi_i^{(+)}\rangle. \quad (2)$$

Solve for $T_{fi} \equiv \langle k_f \phi_f^{(\lambda)} | V | \psi_i^{(+)} \rangle$ at a total energy $E$

$$\langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle = \langle k_f \phi_f^{(\lambda)} | V | \phi_i^{(\lambda)} k_i \rangle$$

$$+ \sum_{n=1}^{N} \int d^3 k \frac{\langle k_f \phi_f^{(\lambda)} | V | \phi_n^{(\lambda)} k \rangle \langle k \phi_n^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle}{E + i0 - \varepsilon_n^{(\lambda)} - k^2 / 2}. \quad (3)$$

Have step-function behaviour:

$$\langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle \approx 0 \text{ for } \varepsilon_f^{(\lambda)} > k_f^2 / 2.$$
Scattering:

Electron-atom wavefunction is expanded as

$$|\psi^{(+)}_i\rangle \approx A \sum_{n=1}^{N} |\phi^{(\lambda)}_n\rangle \langle \phi^{(\lambda)}_n | \psi^{(+)}_i\rangle \equiv A l_N |\psi^{(+)}_i\rangle.$$  \hspace{1cm} (2)

Solve for $T_{fi} \equiv \langle k_f \phi^{(\lambda)}_f | V | \psi^{(+)}_i\rangle$ at a total energy $E$

$$\langle k_f \phi^{(\lambda)}_f | T | \phi^{(\lambda)}_i k_i \rangle = \langle k_f \phi^{(\lambda)}_f | V | \phi^{(\lambda)}_i k_i \rangle$$

$$+ \sum_{n=1}^{N} \int d^3k \frac{\langle k_f \phi^{(\lambda)}_f | V | \phi^{(\lambda)}_n k \rangle \langle k \phi^{(\lambda)}_n | T | \phi^{(\lambda)}_i k_i \rangle}{E + i0 - \varepsilon^{(\lambda)}_n - k^2/2}. \hspace{1cm} (3)$$

Have step-function behaviour:

$$\langle k_f \phi^{(\lambda)}_f | T | \phi^{(\lambda)}_i k_i \rangle \approx 0 \text{ for } \varepsilon^{(\lambda)}_f > k^2_f/2.$$
Define scattering amplitude $f_{fi}$ via

$$
\langle \Phi_f^{(-)} | \overset{\leftarrow}{H} - E | \Psi_i^{(+)} \rangle \approx \langle k_f \phi_f^{(-)} | l_N (\overset{\leftarrow}{H} - E) A l_N | \psi_i^{(+)} \rangle = \langle \phi_f^{(-)} | \phi_f^{(\lambda)} \rangle \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle ,
$$

where $\varepsilon_f = \varepsilon_f^{(\lambda)}$ ensured $\langle \phi_f^{(-)} | l_N = \langle \phi_f^{(-)} |$.

- **Discrete excitation** $[\varepsilon_f < 0, \langle \phi_f^{(-)} | \phi_f^{(\lambda)} \rangle = 1]$:

  $$
f_{fi}^{(N)} (k_f) = \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle ,
$$

- **Ionisation** $[\varepsilon_f = q_f^2 / 2$, with $\langle \phi_f^{(-)} | \equiv \langle q_f^{(-)} |$] :

  $$
f_{i}^{(N)} (q_f, k_f) = \langle q_f^{(-)} | \phi_f^{(\lambda)} \rangle \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle ,
$$
Define scattering amplitude $f_{fi}$ via

$$\langle \Phi_f^{(-)} | H - E | \Psi_i^{(+)} \rangle \approx \langle k_f \phi_f^{(-)} | l_N (H - E) A l_N | \psi_i^{(+)} \rangle$$

$$= \langle \phi_f^{(-)} | \phi_f^{(\lambda)} \rangle \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle,$$

where $\varepsilon_f = \varepsilon_f^{(\lambda)}$ ensured $\langle \phi_f^{(-)} | l_N = \langle \phi_f^{(-)} |$.

Discrete excitation $[\varepsilon_f < 0, \langle \phi_f^{(-)} | \phi_f^{(\lambda)} \rangle = 1]$:

$$f_{fi}^{(N)}(k_f) = \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle,$$

Ionisation $[\varepsilon_f = q_f^2 / 2, \text{with } \langle \phi_f^{(-)} | \equiv \langle q_f^{(-)} |$]

$$f_i^{(N)}(q_f, k_f) = \langle q_f^{(-)} | \phi_f^{(\lambda)} \rangle \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle,$$
Define scattering amplitude \( f_{fi} \) via

\[
\langle \Phi_f^{(-)} | \overset{→}{H} - E | \Psi_i^{(+)} \rangle \approx \langle k_f \phi_f^{(-)} | I_N(\overset{→}{H} - E) A I_N | \psi_i^{(+)} \rangle
= \langle \phi_f^{(-)} | \phi_f^{(\lambda)} \rangle \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle,
\]

where \( \varepsilon_f = \varepsilon_f^{(\lambda)} \) ensured \( \langle \phi_f^{(-)} | I_N = \langle \phi_f^{(-)} | \).

- **Discrete excitation** \( \left[ \varepsilon_f < 0, \langle \phi_f^{(-)} | \phi_f^{(\lambda)} \rangle = 1 \right] : \)

\[
f_{fi}^{(N)} (k_f) = \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle,
\]

- **Ionisation** \( \left[ \varepsilon_f = q_f^2 / 2, \text{ with } \langle \phi_f^{(-)} | \equiv \langle q_f^{(-)} | \right] : \)

\[
f_{i}^{(N)} (q_f, k_f) = \langle q_f^{(-)} | \phi_f^{(\lambda)} \rangle \langle k_f \phi_f^{(\lambda)} | T | \phi_i^{(\lambda)} k_i \rangle,
\]
Photoionisation of atom $A$ in state $\psi_0$:

- We solve (3) to yield $\langle k_f^(-) \phi_f^\lambda | T | \phi_n^\lambda k^+ \rangle$ for electron scattering on $A^+$, write

$$\langle \psi_f^(-) | = \langle k_f^(-) \phi_f^\lambda | + \sum_{n=1}^{N} \int d^3 k \frac{\langle k_f^(-) \phi_f^\lambda | T | \phi_n^\lambda k^+ \rangle \langle \phi_n^\lambda k^+ |}{E + i0 - \varepsilon_n^\lambda - k^2 / 2},$$

and evaluate $\langle \psi_f^(-) | D | \psi_0 \rangle$.

- Single photoionisation: use $\langle \psi_f^(-) | D | \psi_0 \rangle$ for $\varepsilon_f < 0$.
- Double photoionisation: use $\langle q_f^(-) \phi_f^\lambda | \psi_f^(-) | D | \psi_0 \rangle$ for $q_f^2 / 2 = \varepsilon_f > 0$. 
Photoionisation of atom $A$ in state $\Psi_0$:

- We solve (3) to yield $\langle k_f^- \phi_f^\lambda | T | \phi_n^\lambda k^+ \rangle$ for electron scattering on $A^+$, write

$$
\langle \psi_f^- | = \langle k_f^- \phi_f^\lambda | + \sum_{n=1}^N \int d^3k \frac{\langle k_f^- \phi_f^\lambda | T | \phi_n^\lambda k^+ \rangle \langle \phi_n^\lambda k^+ |}{E + i0 - \epsilon_n^\lambda - k^2/2},
$$

and evaluate $\langle \psi_f^- | D | \psi_0 \rangle$.

- Single photoionisation: use $\langle \psi_f^- | D | \psi_0 \rangle$ for $\epsilon_f < 0$.

- Double photoionisation: use $\langle q_f^- | \phi_f^\lambda \rangle \langle \psi_f^- | D | \psi_0 \rangle$ for $q_f^2/2 = \epsilon_f > 0$.
Two-centre problems: positron or proton impact on atoms

$$\Psi(R, r) \approx \sum_{n=1}^{N} \phi^{N}_{n}(r)f^{N}_{n}(R) + \sum_{n=1}^{N'} \phi'^{N'}_{n}(x)f'^{N'}_{n}(X)$$
Nonrelativistic CCC theory

• $e^-\cdot H$ S-wave model: excitation and total ionisation

![Graphs showing cross section vs. projectile energy for different states (1s, 2s, 3s) for electron-impact ionisation of $H$.]

Poet 1978
CCC(30)
CCC(10)
CCC(5)

$\sigma_0^2$
Nonrelativistic CCC theory

Convergence studies

electron-impact excitation at 3 Ry

Two graphs show the cross section in atomic units squared ($a_0^2$) against energy in Rydbergs (Ry). The graphs compare the triplet and singlet states for different CCC methods: CCC(10), CCC(20), and CCC(30). The cross sections are plotted on a logarithmic scale for both axes.
Nonrelativistic CCC theory

Convergence studies

electron-impact ionisation $\frac{d\sigma_i}{de}(e)$ at 3 Ry
Can estimate true SDCS from $\sigma_{i}^{\text{ion}}$ and $\frac{d\sigma_{i}}{de}(E/2)$.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{plot.png}
\caption{Comparison of singlet FDM, CCC, and estimate for cross section vs. secondary energy.}
\end{figure}
e\(^+\)-H S-wave model: H(1S), Ps(1S) and breakup

\[\text{(plots showing cross sections)}\]
e\(^+\)-H S-wave model: H(1S), Ps(1S) and breakup

\[\text{Cross section} \ (\pi a_0^2)\]

- **H(1S)**
  - CC(1,1)
  - CC(2,2)
  - CC(5,5)

- **Ps(1S)**
  - CC(1,1)
  - CC(2,2)
  - CC(5,5)
**Nonrelativistic CCC theory**

**convergence studies**

- $e^+\text{-H S-wave model: H(1S), Ps(1S) and breakup}$

---

**Graphs:**

- Cross section $(\pi a_0^2)$ vs. positron energy (eV)
- **H(1S)**
  - $CC(15,1)$
  - $CC(15,5)$

- **Ps(1S)**
  - $CC(15,1)$
  - $CC(15,5)$
Nonrelativistic CCC theory

convergence studies

\( e^+ - H \) S-wave model: H(1S), Ps(1S) and breakup

Cross section \((\pi a_0^2)\) for H(1S) and Ps(1S) with CCC methods.

Igor Bray <I.Bray@curtin.edu.au>

CCC method for electron-impact ionisation of ions
e⁺-H S-wave model: H(1S), Ps(1S) and breakup

![Graph showing cross sections for breakup (H,Ps) and breakup (Ps)]
Relativistic CCC theory

- Dirac Hamiltonian does not have a lowest energy state, but a negative-energy continuum.
- We diagonalise following Grant and Quiney, PRA 62 022508 (2000).
Relativistic CCC theory

coupled Lippmann-Schwinger equations

\[ T_{fi}^{++}(k_f, k_i) = V_{fi}^{++}(k_f, k_i) + \sum_{n=1}^{N} \int d^3k \frac{V_{fn}^{++}(k_f, k) T_{ni}^{++}(k, k_i)}{E + i0 - \epsilon_n^{(\lambda)} - \epsilon_k} \]

\[ + \sum_{n=1}^{N} \int d^3k \frac{V_{fn}^{+-}(k_f, k) T_{ni}^{-+}(k, k_i)}{E + i0 - \epsilon_n^{(\lambda)} + \epsilon_k}, \]

\[ T_{fi}^{-+}(k_f, k_i) = V_{fi}^{-+}(k_f, k_i) + \sum_{n=1}^{N} \int d^3k \frac{V_{fn}^{-+}(k_f, k) T_{ni}^{++}(k, k_i)}{E + i0 - \epsilon_n^{(\lambda)} - \epsilon_k} \]

\[ + \sum_{n=1}^{N} \int d^3k \frac{V_{fn}^{--}(k_f, k) T_{ni}^{-+}(k, k_i)}{E + i0 - \epsilon_n^{(\lambda)} + \epsilon_k}, \]

where “+/−” corresponds to electrons/positrons.
Relativistic CCC theory
Breit and Møller corrections

- The Breit correction is

\[ V_{12} = \frac{1}{r_{12}} \left[ 1 - \alpha_1 \cdot \alpha_2 + \frac{1}{2} (\alpha_1 \cdot p_1 \alpha_2 \cdot p_2) r_{12}^2 \right] \]

\( \alpha_i \) are Dirac matrices, \( p_i \) the electron momenta, and \( r_{12} \) is the distance between the two electrons.

- The Møller correction is

\[ V_{12} = \frac{1}{r_{12}} (1 - \alpha_1 \cdot \alpha_2) \exp(iKr_{12}), \]

where \( K = |E - E'|/c \).
H-like targets

Electron-impact ionisation cross section

\[ \sigma_i = \int_0^E d\varepsilon \frac{d\sigma_i}{d\varepsilon}(\varepsilon). \]

![Graph showing e-H total ionisation cross section vs total energy.](image-url)
25 eV e-H singly differential cross section $\frac{d\sigma_i}{d\epsilon}(\epsilon)$
25 eV e-H doubly differential cross sections $\frac{d^2\sigma_i}{dE d\Omega}(\theta)$

- $E_s = 2$ eV
- $E_s = 3$ eV
- $E_s = 4$ eV
- $E_s = 5.7$ eV

Scattering angle (deg) vs. cross section ($10^{-19}$ cm$^2$sr$^{-1}$eV$^{-1}$).

- Shyn (1992)
- ECS
- CCC

Igor Bray <I.Bray@curtin.edu.au>

CCC method for electron-impact ionisation of ions
25 eV e-H \( E_A = E_B = 5.7 \) eV coplanar FDCS

\[
\theta_{AB} = 80^\circ
\]

- Roeder
- CCC
- ECS

\[
\theta_{AB} = 120^\circ
\]

\[
\theta_{AB} = 100^\circ
\]

\[
\theta_{AB} = 150^\circ
\]
electron-impact ionisation of B$^{4+}$

![Graph showing electron-impact ionisation cross section against electron energy for B$^{4+}$ ions. The graph includes data points and lines for various theoretical models: Aichele et al, DWBA(LANL), CCC, CCC(S=1), and CCC(S=0). The x-axis represents electron energy in eV, ranging from 500 to 3000, and the y-axis represents cross section in Mb (Mega-barns), ranging from 0 to 0.3. The graph compares these models against experimental data.](image-url)
Introduction
Nonrelativistic CCC theory
Relativistic CCC theory
Electron-impact ionisation
Concluding remarks

H-like targets
He-like targets
Na-like targets
Mg-like targets

electron-impact ionisation of Ca^{19+}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure.png}
\caption{Comparison of cross sections for electron-impact ionisation of Ca^{19+} using different methods.}
\end{figure}

Igor Bray <I.Bray@curtin.edu.au>
CCC method for electron-impact ionisation of ions
Introduction
Nonrelativistic CCC theory
Relativistic CCC theory
Electron-impact ionisation
Concluding remarks

H-like targets
He-like targets
Na-like targets
Mg-like targets

• electron-impact ionisation of Zn^{29+}

<table>
<thead>
<tr>
<th>electron energy (eV)</th>
<th>cross section (Mb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20000</td>
<td>0.0003</td>
</tr>
<tr>
<td>40000</td>
<td>0.00025</td>
</tr>
<tr>
<td>60000</td>
<td>0.0002</td>
</tr>
<tr>
<td>80000</td>
<td>0.00015</td>
</tr>
<tr>
<td>100000</td>
<td>0.0001</td>
</tr>
</tbody>
</table>

- DWBA(LANL)
- RCCC
- CCC
- CCC(S=0)
- CCC(S=1)

Igor Bray <I.Bray@curtin.edu.au>
electron-impact ionisation of $W^{73+}$

![Graph showing electron-impact ionisation of $W^{73+}$](image-url)
**Introduction**

- Nonrelativistic CCC theory
- Relativistic CCC theory
- Electron-impact ionisation
- Concluding remarks

**H-like targets**

- He-like targets
- Na-like targets
- Mg-like targets

**electron-impact ionisation of U$$^{91+}$$**

![Graph showing cross section vs. electron energy for electron-impact ionisation of U$$^{91+}$$.](image)

- **Our Coulomb Born**
- **Fontes Coulomb Born**
- **Our Moller Born**
- **Fontes Moller Born**
- **full RCCC Coulomb**
- **Experiment: Marrs et al.**

<table>
<thead>
<tr>
<th>electron energy (keV)</th>
<th>cross section ($10^{-24}$ cm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0.0</td>
</tr>
<tr>
<td>200</td>
<td>0.5</td>
</tr>
<tr>
<td>300</td>
<td>1.0</td>
</tr>
<tr>
<td>400</td>
<td>1.5</td>
</tr>
<tr>
<td>500</td>
<td>2.0</td>
</tr>
<tr>
<td>600</td>
<td>2.5</td>
</tr>
<tr>
<td>700</td>
<td>3.0</td>
</tr>
<tr>
<td>800</td>
<td>4.0</td>
</tr>
</tbody>
</table>

*Igor Bray <I.Bray@curtin.edu.au>*

**CCC method for electron-impact ionisation of ions**
Electron-impact ionisation
He-like targets

**e-He total ionisation cross sections**

- **1-1-S**
  - CCC, PRA(1995)

- **2-3-S**
  - Exp, JPB(1976)
  - CCC, JPB(2003)
  - CCC(S=0)
  - CCC(S=1)
  - Exp, PRA(1989)

Igor Bray <I.Bray@curtin.edu.au>

CCC method for electron-impact ionisation of ions
e-Li$^+$ total ionisation cross sections

![Graph showing e-Li$^+$ total ionisation cross sections](image)
e-B\(^3^+\) total ionisation cross sections

![Graph showing total ionisation cross sections for e-B\(^3^+\) as function of energy.](image)

- Overview scan
- Present experimental data
- CCC 89.5% g.c. + 10.5% m.s.
e-O$^{6+}$ total ionisation cross sections

- CCC
- CCC(S=0.5)
- CCC(S=1.5)
- DWBA(LANL)

Cross section (10$^{-21}$ cm$^2$) vs. projectile energy (eV)

Igor Bray <I.Bray@curtin.edu.au>

CCC method for electron-impact ionisation of ions
Electron-impact ionisation

Na-like targets

- e-Na total ionisation cross sections

![Graph showing e-Na total ionisation cross sections for different models and experimental data.](image-url)
e-Na $E_A = E_B$ eV coplanar fully differential Xsecs

- $E_A = E_B = 3$ eV
- $E_A = E_B = 5$ eV
- $E_A = E_B = 10$ eV
- $E_A = E_B = 15$ eV
- $E_A = E_B = 20$ eV
- $E_A = E_B = 30$ eV

Murray
CCC

fully differential cross section (a.u.)

scattering angle $\theta_A = -\theta_B$ (deg)
**e-Si\(^{3+}\) total ionisation cross sections**

![Graph showing total ionisation cross sections for e-Si\(^{3+}\) for different theories: DWBA(LANL), CCC, CCC(S=0), and CCC(S=1). The graph plots cross section (10\(^{-17}\) cm\(^2\)) against projectile energy (eV).]
e-Cl\(^{6+}\) total ionisation cross sections

![Graph showing total ionisation cross sections for e-Cl\(^{6+}\) as a function of projectile energy (eV). The graph compares different theoretical methods: DWBA (LANL), CCC, CCC (S=0), and CCC (S=1).]
e-$\text{Ar}^{7+}$ total ionisation cross sections

![Graph showing total ionisation cross sections for e-$\text{Ar}^{7+}$ as a function of projectile energy.]}
Electron-impact ionisation
Mg-like targets

**e-Mg total ionisation cross sections**

![Graph showing e-Mg(3^3S) TICS cross section versus electron energy (eV). The graph includes data points for experimental (exp, PRA 1998), CCC, and DWBA (LANL) methods.](image-url)
e-Mg fully differential ionisation

\[ E_A = E_B = 15\text{eV} \]

\[ E_A = E_B = 20\text{eV} \]

\[ E_A = E_B = 25\text{eV} \]

\[ E_A = E_B = 30\text{eV} \]

Cross section (a.u.)

scattering angle \( \theta_A = -\theta_B \) (deg)
**e-Si$^{2+}$** total ionisation cross sections

![Graph showing the total ionisation cross sections for e-Si$^{2+}$ as a function of projectile energy (eV). The graph compares TICS, DWBA(LANL), and CCC methods. The CCC method shows a peak at a projectile energy of around 100 eV, then decreases gradually.]
**e-Cl$^{5+}$** total ionisation cross sections

![Graph showing total ionisation cross sections for e-Cl$^{5+}$]

- **e-Cl$^{5+}$ TICS**
  - DWBA (LANL)
  - CCC

**Cross section (10^{-17} \text{cm}^2)** vs. **projectile energy (eV)**
**e-Ar$^{6+}$ total ionisation cross sections**

The graph shows the total ionisation cross sections for e-Ar$^{6+}$ ions as a function of projectile energy in eV. The data is compared with different theoretical models:

- DWBA (Differential Wave Barrier Approximation)
- CCC (Coupled Channels Coupling)

The cross sections are presented in units of $10^{-17}$ cm$^2$. The graph indicates that the CCC model generally reproduces the experimental data well, especially at lower projectile energies. The DWBA model, on the other hand, tends to overestimate the cross sections at higher energies.

Igor Bray <I.Bray@curtin.edu.au>  
CCC method for electron-impact ionisation of ions
Concluding remarks

- Have found that for quasi one-electron targets spin asymmetries are large irrespective of ionic charge.
- Generally very good agreement of CCC and DWBA as the ionic charge increases.
- Presently we are extending CCC to:
  - positron collisions with quasi one- and two-electron targets
  - multi-channel proton collisions
  - more complicated targets, such as inert gases and molecules.
Concluding remarks

- Have found that for quasi one-electron targets spin asymmetries are large irrespective of ionic charge.
- Generally very good agreement of CCC and DWBA as the ionic charge increases.
- Presently we are extending CCC to:
  - positron collisions with quasi one- and two-electron targets
  - multi-channel proton collisions
  - more complicated targets, such as inert gases and molecules.