The low-energy inelastic scattering of electrons by atomic systems

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Collaboration:

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- ITM-AMNS TF
- ADAS

Electron and photon interactions with atoms and ions:

RMATX I and BPRM, and FARM in the external region
RMATX II for electron excitation (non-relativistic) and FARM
R-matrix Floquet and LIDS for radiative damping effect in DR
GRASP and DARC (full relativistic)
Cowan’s suite code
Advanced graph database for data representation and data processing

It is a new kind of data representation that allows for parallel computing due to multiple storage servers employed combined with data storage in binary files. Furthermore, storage space is allocated when needed, thus allowing to gradually expanding the capacity while the system is online, by either adding new storage servers or adding disks in existing ones; It is also implemented a built-in security layer.

Relativistic and Non-relativistic R-matrix Codes for Atomic Processes, Currently used on our ATOMIC Computing facility
Outline:

• Theoretical models and numerical methods: Application to the electron collision with C atoms

  a) Atomic data calculation (overview on the existing target models)
  b) Electron collision data (comparison between published cross sections, and new results)
  c) Resonance phenomena in collisions of electrons with the C IV ion: interference effects between DR and RR on PR cross section.

• Comparison of perturbative (BPRM) and non-perturbative (MCDF-EAL) predictions for fine-structure splitting in Ar III ion

  a) Atomic data calculation (comparison with other works)
  b) Selected electron collision data

• Conclusions
Earlier works:

\( n = 2 \)
- R-matrix (Le Dourneuf 1976, Le Dourneuf et al. 1977)

\( n \leq 3 \)
- Relativistic R-matrix method (LS > pair coupling) (Johnson, Burke, Kingston 1987)
- R-matrix (LS) (Dunseath et al, 1997) (28 target states)

\( n \leq 4 \)
- R-matrix (LS) (Dunseath et al, JPB 1997)- 48 target states
- \( B \)-spline R-matrix (Zatsarinny & Bartschart PRA (2005)) – 28 target states
- Momentum-space coupled-channels optical (CCO) method (Liu, Wang, Zhou, JPB 2006)
Study of the electron collision with C atoms
Methods and Target models

The most detailed calculations:

3. Dunseath et.al. (JPB 1997): R-matrix method and code (RMATXI), and two independent calculations:

   I. \( n \leq 3 \) (28 target states)
   II. \( n \leq 4 \) (48 target states)

   The standard R-matrix method does not treat the continuum of target.

4. Zatsarinny et.al. (PRA 2005)) use the B- spline R-matrix method to calculate the excitation cross sections. MCHF method is used to describe the wavefunctions of target states, and the B- spline bases are employed in the close coupling expansion to mimic the continuum states. 28 target states and 8 pseudostates to account for the target continuum.

5. Liu et.al. (JPB 2006) 12 states are included in coupled-channels optical calculation. They are described by the single configuration Hartree-Fock approximation. The continuum optical potential in the \( ^3\!P_0 - ^3\!P_0, ^3\!P_0 - ^3\!P_1 \) and \( ^3\!P_1 - ^3\!P_1 \) couplings have been included.
Cross sections as function of incident electron energy for the electron-impact excitation of the 2p3s, 2p3p and 2p3d transitions from the $1s^22s^22p^2{}^3P$ ground state of carbon.

Comparing existing data: a) all results agree well in shape; b) large discrepancies in magnitude exist among all these calculations: Dunseath’s result is 32% higher than the calculation of B-spline R-matrix method, and the results of CCO method are 18% lower than the calculation of B-spline R-matrix method (Liu et al. 2006)
The importance of including CI wavefunctions both in the target-state expansion and in the (N+1)-electron quadratically integrable function expansion is investigated;

Electron correlation effects are explored by carrying out separate calculations with and without the configurations:

- $2s^2p^3$, $2s2p^2nl$ ($n=3,4$), $2p^4$ in the target state expansion,
- $2s^22p^3$, $2s2p^4$, $2s2p^3nl$ ($n=3,4$) in the (N+1)-electron wavefunction.
Collision strengths for the first $^3P - ^1D$ transition for the $^4P^0$ symmetry. We compare and contrast the collision strengths as output from two different calculations where the terms arising from the $1s^22s^22pnl$ manifolds, and those arising from $1s^22s^22pnl$ and $2s2p^3$ and $2p^4$ manifolds are, respectively, included into the R-matrix expansion.
C.T. Johnson, P.G. Burke and A.E. Kingston (JPB 1987): **Target state model:** 1s, 2s, 2p, 3s, 3p, 3d bound radial orbitals, \( ^3\text{P}_e \), \( ^1\text{D}_e \), \( ^1\text{S}_e \) and three pseudostates \( ^3\text{S}_0 \), \( ^3\text{P}_0 \) and \( ^3\text{D}_0 \) to account for short-range correlation and polarisation effects.
Collision strengths for $^3P_0 - ^1D_2$ with (red) and without (black) $^2p^4$
Effect of quantum interference between DR and RR on photo-recombination cross section: Application to C^3+

- PR gives resonances in electron-collision cross section
- Our precursory work (POP 2005) on DR of Li-like into Be-like C ions gives accurate position and width for resonant states. The model uses RMF theory and code and its extension to LIDS phenomenon;

\[ e^- + A_i^{n+} \xrightarrow{A_j^{(n-1)+} + h\nu} e^- + A_j^{n+} \rightarrow (A_i^{(n-1)})^{**} \]

\[ e^- + A_i^{n+} \rightarrow (A_i^{(n-1)})^{**} \]

\[ \sigma_{if}^{PR}(\varepsilon) = \sigma_{if}^{RR}(\varepsilon) + \sigma_{idf}^{DR}(\varepsilon) + \sigma_{idf}^{int}(\varepsilon) \]

\[ \sigma_{RR}(\varepsilon) = \left( \frac{g_i}{g_u} \right) \frac{\omega_{tune}}{\varepsilon m_e c^2} \sigma_{pl}(\omega_{tune}) \]
Laser-induced degenerate states in Li-like C ions (RMF)

The motion of the complex energies in the complex plane as function of the field intensity for different frequencies and atomic parameters; the critical region where a crossing (or a avoiding crossing) of trajectories occurs.

\[
X^{Z+}[1s^2 2s(2S^e)] + e^- \quad \downarrow \quad X^{(Z-1)^*}[1s^2 2p n^l(1P^0)]
\]

\[
h\nu \quad \downarrow \quad X^{(Z-1)^*}[1s^2 2s n^l(1S^0)]
\]

\[
2E_{1,2} = E_a + E_g - \omega - i(\Gamma_a + I\gamma) / 2 \pm \Omega
\]

\[
\Omega = \{[d - i(\Gamma_a - I\gamma) / 2]^2 + \Gamma_a I\gamma [q - i]^2\}^{1/2}
\]
• Results are shown for series of resonances, of type $^1P_0$, which are allowed in LS coupling.

• 2pns – 2sns transitions
• $n = 5, 6, 7, 8, 9, 10, 11, 12$
• QDT & MPI

$$L_d(\epsilon) = \frac{\Gamma(d)/2\pi}{(\epsilon - \omega_{nue})^2 + \left(\frac{\Gamma(d)}{2}\right)^2}$$

$$\sigma_{idf}^{\text{int}}(\epsilon) = \frac{4}{\hbar A_{di}^q} \left[ (\epsilon - \omega_{nue}) \left( \frac{1}{Q_{idf}} \right) \right] \sigma_{idf}^{\text{DR}}(\epsilon)$$

$$\sigma_{idf}^{\text{DR}}(\epsilon) = \frac{(2\pi\hbar)^3}{8\pi n \epsilon} \frac{(2J_d + 1)}{2(2J_i + 1)} A_{di}^q L_d(\epsilon) B_{df}^D$$

Stancalie, LPB 2013
Electron-scattering by the Ar III ion: $1s^22s^22p^63s^23p^4(3P)$

RMATRXI: BPRM with FARM in the external region: $0 \leq J \leq 7$, $n < 4$, $0 \leq L \leq 9$, $(2S+1)=1,3,5$

Two ‘model’ calculations to stabilise the the order of the levels (odd or even):

A: even: $\{3s^23p^4, 3p^6, 3s3p^43d, 3s^23p^23d^2, 3p^43d^2\}$ giving rise to 126 fine structure levels;
   odd: $\{3s3p^5, 3s^23p^33d, 3p^53d, 3p^3d^2 \text{ and } 3s^23p^3d^3\}$ which give rise to 184 levels

B: In the second model calculation: $3s^23p$, $3s3p^5$, $3s^23p^33d$ and $3p^6$. 24 LS states with a maximum of around 156 channels for each LS$\pi$ symmetry. C.I. was limited to single and double excitations within the $n = 3$ complex.

MCDF-EAL + QED in GRASP with DARC for collision calculation: $J^\pi \leq 0^\pm, 1^\pm, 2^\pm, 3^-, 4^-, 5^-$

- $\{3s^23p^4, 3s3p^5, 3s^23p^23d^2 \text{ and } 3p^6\}$ which give 48 fine structure levels.
- To stabilise the order of levels, an initial analysis on each parity has been done:

A (even): $\{3s^23p^4, 3p^6, 3s3p^43d, 3s^23p^23d^2, 3p^43d^2, 3s^23p^34p, 3s^23p^34f, 3p^54f\}$

B (odd): $\{3s3p^5, 3s^23p^33d, 3p^53d, 3s^23p^33d^2, 3s^23p^3d^3, 3s^23p^34s\}$

$\Delta n = 0$, $n = 3$.

Stancalie, et al. EPJD (2012)
Electron-scattering by the Ar III ion: $1s^22s^22p^63s^23p^4(^3P)$

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$3s^23p^4(^3P_{2}-^3P_{1})$

$3s^23p^4(^3P_{1}-^3P_{0})$

$3s^23p^4(^1D_{2}-^1S_{0})$
Conclusions

- In the electron scattering by atomic carbon since the collision models applied are very closed, the differences in the resulting cross sections and collision strengths reflect the differences in the target description;

- The importance of including CI wavefunctions both in the target-state expansion and in the (N+1)-electron quadratically, integrable function expansion has been investigated.

- We have explored the role of configuration interactions allowing for distortion of the initial-state and excited-state orbitals (1p-1h resonances). In the first step of our calculation we chose the single-particle states such that the corresponding (bound) energies agree with the experiment. In the second step, the correlation effects were evaluated. The largest differences in cross section results were found for the dominant transitions of the form 1s\(^2\)2s\(^2\)2p\(^2\) – 1s\(^2\)2s2p\(^3\) in case of carbon.

- PR process gives resonances in the electron-collision cross section. We have determined PR cross sections for C IV ion accounting for the interference between DR and RR processes;

- Independent calculation of the electron scattering by Ar III ion has been carried out. Fine structure splitting calculation has been done using perturbative (BPRM) and non-perturbative (MCDF-EAL) approach.
Thank you!