Ion-impact Excitation for High Precision GCR: Improvements of the Semi-classical, Impact Parameter Approach

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2 October 2015
INAF — Osservatorio Astrofisico di Catania
Motivation: Metastable, Fine-structure Transitions

- As previously explained (see GCR presentation by A. Giunta), \(\text{i}c\)-resolved GCR will require rate coefficients for transitions between the fine-structure levels of metastable terms in an ion — e.g. circled levels in figure.

- Necessarily, the transitions will be of the **quadrupole (E2)** type: dipole excitation is excluded by parity conservation within a term.

- The relatively small energy level differences mean ion-impact excitation can become significant — next slide.
Electron-impact vs. Ion-impact

- Discrepancies in the general structure of electron and ion impact cross-sections as well as where the thermal distributions of the colliding species lie explain why ion-impact favours small energy level differences.

- Increased projectile ion speed distributions can also help: at ITER, we will have ion temperatures $T_i \sim 8$ keV, fast fusion alphas $E_{\alpha:D-T} = 3.5$ MeV, and ionised neutral beam atoms $E_{NB} \sim 1$ MeV [1].

Working in atomic units (au), $\Delta E/I_H$ is the transition energy, $I_H$ is the ionization potential of hydrogen in the same units as $\Delta E$, and $\sigma$ is the cross-section for the arbitrary transition from the target ion level $i$ to $j$. The temperature, $T$, of both the colliding ion and electron velocity distributions (red blocks) is assumed to be equal.
Calculation Technique

- The relatively large mass, $m_p$, of an ion projectile results in an impractically large number of partial waves in the close-coupling region near the target, meaning a semi-classical approach is appropriate versus a fully quantum mechanical one.

- *Coulomb excitation* as per Alder et al [2]: the ion projectile follows a classical trajectory determined by scattering in a Coulomb field, and the excitation probability of the target is obtained through first-order, time dependent perturbation theory.

- The Coulomb excitation differential cross-section is thus given by:

  $$d\sigma_{i\rightarrow j} = P_{i\rightarrow j}(\theta) \left( \frac{z_t z_p}{E_p} \right)^2 \csc^4(\theta/2) d\Omega,$$

where:

- $P_{i\rightarrow j}(\theta)$ is the transition probability for a given trajectory, and the remainder of the theory will address its specification.
- $z_t, z_p$ are the target and projectile charges, respectively.
- $E_p$ is the geometric mean of the projectile kinetic energy: $E_p = \sqrt{E_{p,i} E_{p,f}}$.
- $\theta$ is the scattering angle in the cms frame.
- The boxed term is the classical Rutherford differential cross-section.

The Transition Probability, $P_{i \rightarrow j}$

- First-order, time-dependent perturbation theory tells us:

$$P_{i \rightarrow j} = \frac{1}{\omega_i} \sum_{M_i M_j} |b_{ij}(t = \infty)|^2 ; \quad b_{ij} = \frac{1}{i\hbar} \int_{-\infty}^{\infty} \langle j | H(t) | i \rangle e^{i\omega t} dt.$$  \hspace{1cm} (2)

- After a great deal of algebra and the use of \( \frac{1}{|r_p - r|} \approx \sum \lambda P_{\lambda}(\hat{r}_p \cdot \hat{r}) r^\lambda / r_p^{\lambda+1} \), we find for the quadrupole case:

$$P_{i \rightarrow j}(E2) = 4m_0 B(E2) z_p^{-2} z_t^{-4} E_{p,i} E_p^2 \sin^4 (\theta/2) \frac{df_{E2}}{d\Omega} (\theta, \xi) ,$$  \hspace{1cm} (3)

where $B(E2)$ is the reduced, quadrupole atomic transition probability that we obtain from our atomic structure calculations, $m_0$ is the reduced mass of the projectile and target, and $\xi$ is the dimensionless, symmetrized adiabaticity parameter: $\xi \propto E_p^{-3/2}$.

$$\frac{df_{E2}}{d\Omega} (\theta, \xi)$$ is the differential excitation cross-section function made up of classical orbital integrals that fall out of the right hand equation in 2; these integrals need to be computed numerically, and a table of pre-computed values due to Alder et al [2] has been employed in numerous computer programs — an area for improvement.
Detailed Considerations and History of $P_{i \to j}$

- Coulomb excitation calculations have a long history, but the subject must be revisited because numerous mistakes have been made when calculating $P_{i \to j}$.
- Penetrating collisions and the strong-coupling region need to be treated correctly, as in the figure.
- Codes due to Bely and Faucher [3] and Bahcall and Wolf [4] both treat penetrating collisions incorrectly, leading to the incorrect high energy scaling of the cross-section.
- Seaton [5] gets this right but does not ensure the correct fall-off of the cross-section.
- Burgess and Tully [6] summarize the mistakes and present a completely corrected form of the theory, but their resulting code has been lost.
Objectives

End Goal

Replace the lost Burgess and Tully [6] semi-classical Coulomb excitation code with our own code that will assimilate fully within the ADAS framework.

- First step: use the proton-impact Bely-Faucher [3] codes as source of initial ion-impact data and make necessary minor modifications as a learning experience and in an effort to mitigate flaws.
- Completed modifications:
  - Generalization to permit any bare nucleus projectile (ie $m_p$ and $z_p$ parameters introduced)
  - Extension of $\frac{df_{E2}}{d\Omega} (\theta, \xi)$ data table: higher mesh density and lower values of $\xi$ (higher $E_p$ values for cross-sections) — more on next slide
  - Incorporation of Bethe limit, $\Omega_{lim}$, from structure calculation for extrapolation of collision data during rate coefficient calculation — two slides forward
Extension of $\frac{df_{E2}}{d\Omega}(\theta, \xi)$ Data Table

- ‘extended’ refers to the use of the extended $\frac{df_{E2}}{d\Omega}(\theta, \xi)$ data table, and ‘coarse’ to the original, limited data table from Alder et al.
- ‘linear’ refers to linear interpolation of the cross-sections between the values obtained using the $\frac{df_{E2}}{d\Omega}(\theta, \xi)$ table, and ‘cubic’ refers to cubic spline interpolation
- In theory, the Bely-Faucher (1970) results should lie on top of our coarse, linear results as these codes should be nearly identical; however, provenance is uncertain
Inclusion of $\Omega_{\text{lim}}$ for Rate Coefficient Calculation

- BFHE = original Bely-Faucher strategy for high energy contribution of cross-section to rate coefficient: $\sigma_{ij}(E_f) \cdot E_f = \text{cons.} = C$ and so $\alpha^{\text{HE}} = C \int e^{-E_i/kT} d(E_i/kT) = C$
- AIHE = fit a line to last collision strength and $\Omega_{\text{lim}}$ and compute improper integrals using analytic form similar to above
- 'Recommended' is extended, cubic, BFHE: use of our extended $\frac{df_{E_2}}{d\Omega}(\theta, \xi)$ data table, cubic spline interpolation of cross-sections during integration, and the BFHE scheme
Projectile Variation

B-like Isoseq: $2s2p^2 \, ^4P_{1/2} \rightarrow 2s2p^2 \, ^4P_{3/2}$

- Change from decreasing function along projectile sequence at lower $T_p$ to increasing function along projectile sequence at higher $T_p$ can be explained by $z_p$ scaling of cross-sections
Variation of Cross-section

B-like Sequence, $2s2p^2 \, ^4P_{1/2} \rightarrow 2s2p^2 \, ^4P_{3/2}$

$\sigma_{jk} \left( \pi a_0^2 \right)$

Projectile Initial Energy, $E_i$ (eV)

Cross-Section, $\sigma_{jk} \left( \pi a_0^2 \right)$

$\text{B-like Sequence, } 2s2p^2 \, ^4P_{1/2} \rightarrow 2s2p^2 \, ^4P_{3/2}$

$zp_1, zp_2, zp_4, zp_8$
Projectile Variation: 3D High T

B-like Isoseq: \(2s2p^2 \, {}^4P_{1/2} \rightarrow 2s2p^2 \, {}^4P_{3/2}\)
Projectile Variation: 3D Low T

B-like Isoseq: $2s2p^2 \,^4P_{1/2} \rightarrow 2s2p^2 \,^4P_{3/2}$
Target Variation

B-like Isoseq: \( 2s2p^2 \, ^4P_{1/2} \rightarrow 2s2p^2 \, ^4P_{3/2} \)

- Decreasing \( \alpha_{i \rightarrow j} \) along target sequence at lower \( T_p \) is likely again due to repulsive effect at threshold.
Concluding Remarks

• We have successfully implemented a set of codes which can calculate ion-impact excitation cross-sections and rate coefficients using the Coulomb excitation approximation.

• Accommodation of any bare nucleus projectile has been achieved, with correct scaling of rate coefficients and cross-sections achieved.

• Expansion of the $\frac{df_{E_2}}{d\Omega}(\theta, \xi)$ data table and incorporation of the Bethe limit for collision strength extrapolation have implemented as improvements upon the Bely-Faucher and in preparation of what will be need to be done with our own re-write.

• Preliminary Generalized Collisional-Radiative (GCR) modelling has shown that ion-impact excitation will indeed have an effect upon metastable populations relevant for spectroscopic modelling.

• The next step will be to implement the full prescription of Burgess and Tully in our own code, correctly dealing with penetrating collisions and ensuring the proper high energy behaviour.


