Medium weight element fine structure GCR modelling and the role of ion impact

Alessandra Giunta, Martin O'Mullane, Matthew Bluteau,
Hugh Summers, Stuart Henderson

Motivation

- Towards intermediate coupling (*ic*) GCR

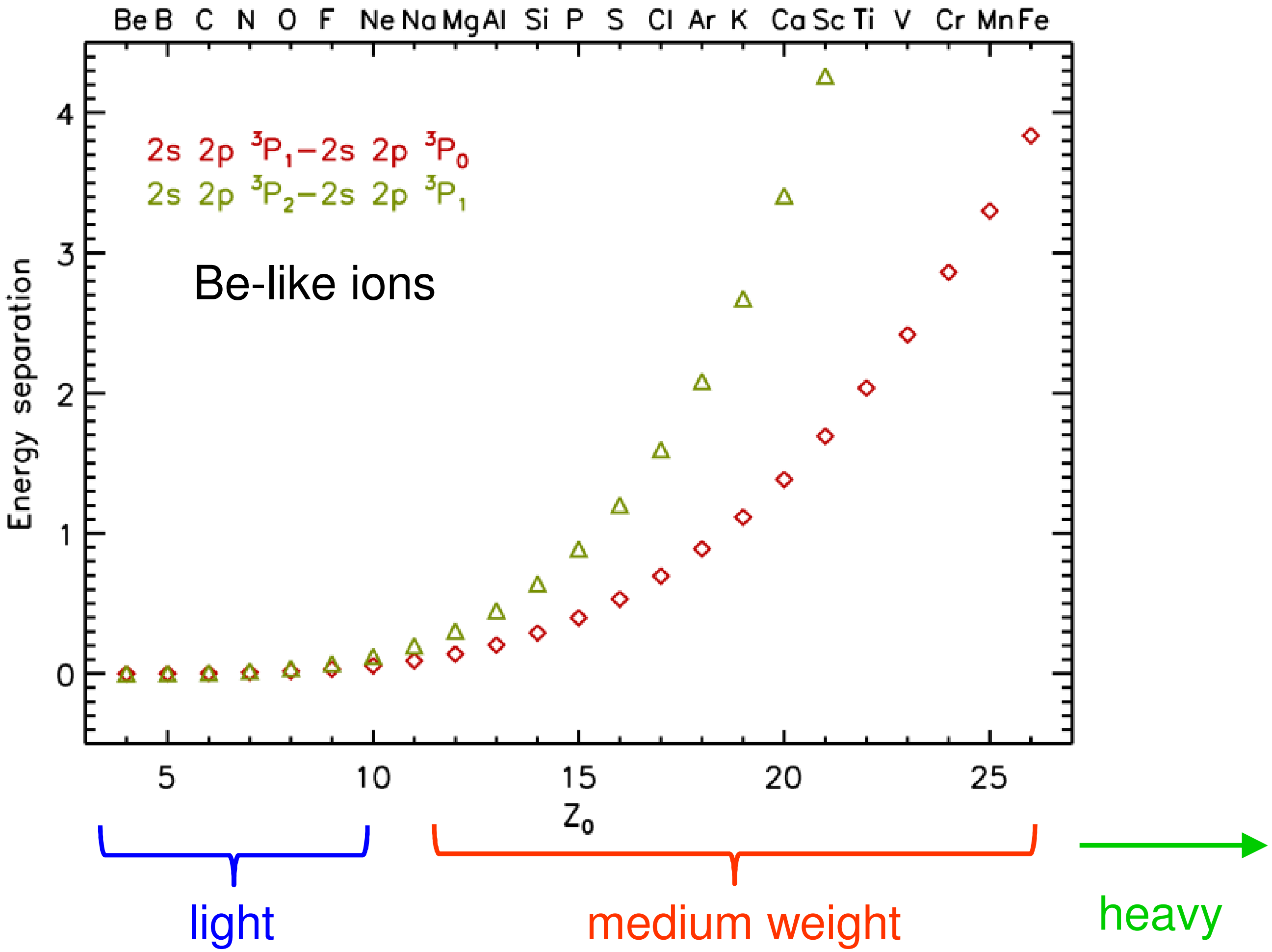
  For medium weight species and more highly ionised ions, term resolved resolution (*ls*) is not appropriate because the fine structure separation within a term becomes significant and the relative populations begin to deviate from statistical.

- Inclusion of ion impact:

  - Ion impact affects transition between close lying levels and so the fine structure.
  - *ic* GCR involves interaction between levels.
  - Level separation increases with Z that is going to medium weight/heavy element ions.

  Ion impact cross sections need to be included in the population calculations.

Fine structure and medium weight species



Generalised Collisional-Radiative modelling

Considering a set of metastable levels or terms X_ρ^{+z} indexed by Greek letters and ordinary excited levels X_i^{+z} indexed by Roman letters, the populations are described by the GCR/CR matrix, where the "script" GCR coefficients give the connection between the metastables within and across ionisation stages.

$$\frac{d}{dt}\begin{bmatrix} N_\mu^{+z-1} \\ N_\rho^{+z} \\ N_i^{+z} \\ N_\nu^{+z+1} \end{bmatrix} = \begin{bmatrix} \mathcal{C}_{\mu\mu'} & N_e\mathcal{R}_{\mu\sigma} & 0 & 0 \\ N_e\mathcal{S}_{\rho\mu'} & C_{\rho\sigma} & C_{\rho j} & N_e r_{\rho\nu'} \\ 0 & C_{i\sigma} & C_{ij} & N_e r_{i\nu'} \\ 0 & N_e S_{\nu\sigma} & N_e S_{\nu j} & \mathcal{C}_{\nu\nu'} \end{bmatrix} \begin{bmatrix} N_{\mu'}^{+z-1} \\ N_\sigma^{+z} \\ N_j^{+z} \\ N_{\nu'}^{+z+1} \end{bmatrix}$$

According to the quasi-static assumption $dN_i^{+z}/dt = 0$ and adopting summation convention on repeated indices:

$$\begin{aligned} \frac{dN_\rho^{+z}}{dt} &= C_{\rho j}N_j^{+z} + C_{\rho\sigma}N_\sigma^{+z} + N_e r_{\rho\nu'}N_{\nu'}^{+z+1} \\ 0 &= C_{i\sigma}N_\sigma^{+z} + C_{ij}N_j^{+z} + N_e r_{i\nu'}N_{\nu'}^{+z+1} \end{aligned}$$

Population calculations: level resolved and ion impact

From the quasi-equilibrium statistical balance the populations of the ordinary excited levels are given by:

$$C_{ij}N_j^{+z} = -C_{i\sigma}N_\sigma^{+z} - N_e r_{i\nu'} N_{\nu'}^{+z+1}$$

where the coefficients include all collisional and radiative contributions:

$$C_{ij} = -A_{j\to i} - N_e q_{j\to i}^{(e)} - \boxed{N_{ion} q_{j\to i}^{(ion)}} \quad i \neq j$$

ion impact

$$C_{ii} = \sum_{j<i} A_{i\to j} + N_e \sum_{j\neq i} q_{i\to j}^{(e)} + \boxed{N_{ion} q_{i\to j}^{(ion)}} + N_e q_i^{(I)}$$

The ion impact shown here, in principle, is ignorable except within metastable fine structure.

GCR coefficients

Considering the metastable level (or term) populations:

$$\frac{dN_{\rho}^{+z}}{dt} = -(N_e S_{CD,\sigma\rightarrow\nu} N_{\sigma}^{+z} + N_e \alpha_{CD,\nu'\rightarrow\rho} N_{\nu'}^{+z+1} + N_e Q_{CD,\sigma\rightarrow\rho} N_{\sigma}^{+z}) + \ldots$$

The effective GCR coefficients are the following:

Effective ionisation coefficient

$$S_{CD,\sigma\rightarrow\nu} = S_{\nu\sigma} - S_{\nu j} C_{ji}^{-1} C_{i\sigma}$$

Effective recombination coefficient

$$\alpha_{CD,\nu'\rightarrow\rho} = r_{\rho\nu'} - C_{\rho j} C_{ji}^{-1} r_{i\nu'}$$

Effective metastable cross-coupling coefficient

$$Q_{CD,\sigma\rightarrow\rho} = (C_{\rho\sigma} - C_{\rho j} C_{ji}^{-1} C_{i\sigma})/N_e$$

Metastable cross-coupling coefficient Q_{CD}

Since the transitions which are readily excited by ions are those between close lying levels, ion impact can be included in the GCR modelling through the metastable cross-coupling coefficient in the form:

$$Q_{CD,\sigma\rightarrow\rho}^{total} \simeq Q_{CD,\sigma\rightarrow\rho}^{(e)} + (N_{ion} q_{\sigma\rightarrow\rho}^{ion})/N_e$$

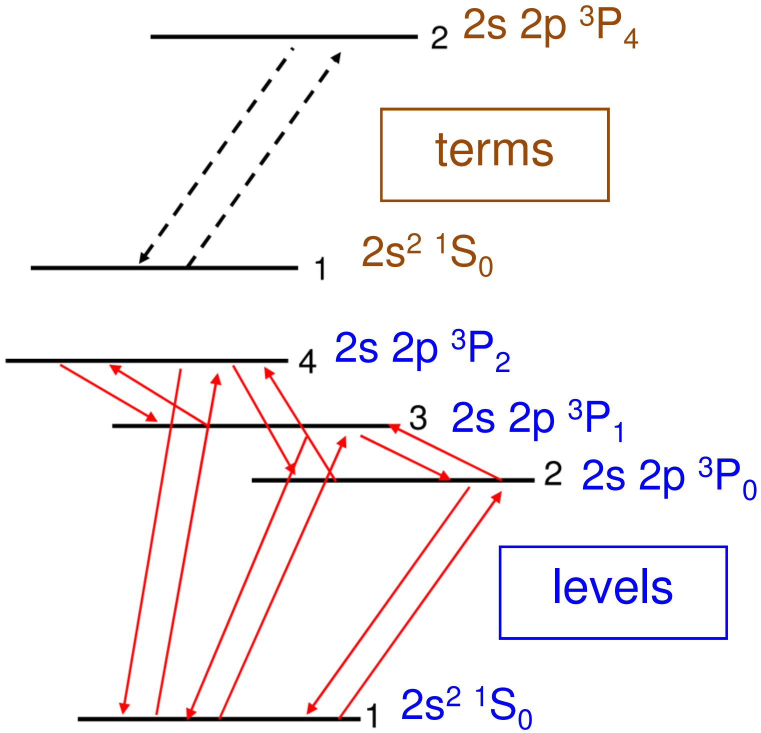
In practice, there may be several ion collider species and so:

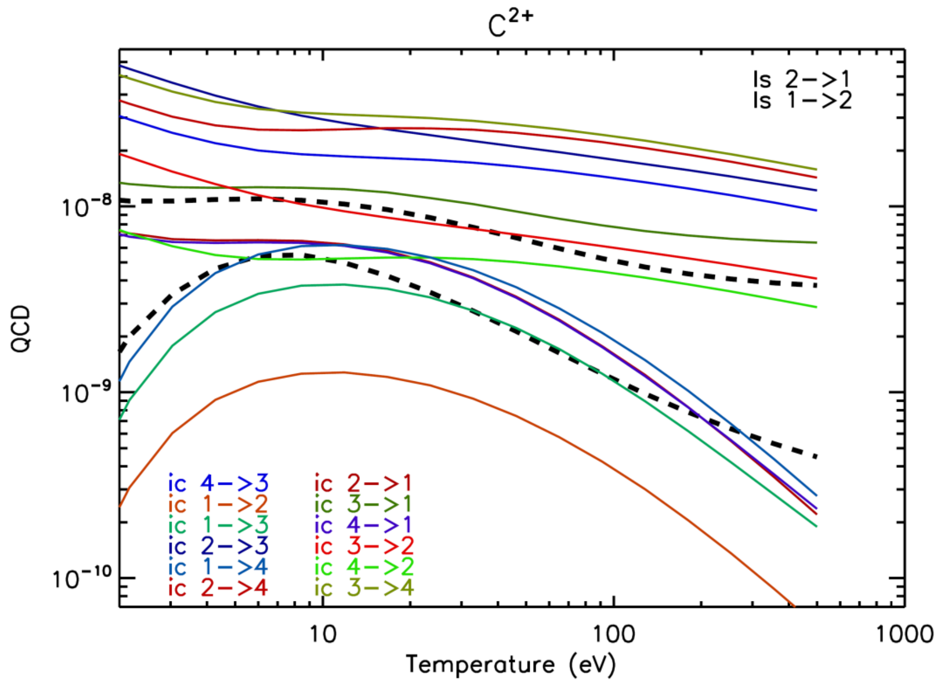
$$Q_{CD,\sigma\rightarrow\rho}^{total} \simeq Q_{CD,\sigma\rightarrow\rho}^{(e)} + \left(\sum_{ion} N_{ion} q_{\sigma\rightarrow\rho}^{ion}\right)/N_e$$

Ion impact rates $q_{\sigma\rightarrow\rho}^{ion}$ for different colliders are archived in the ***adf06*** data files.

Term and level resolved Q_{CD} coefficients

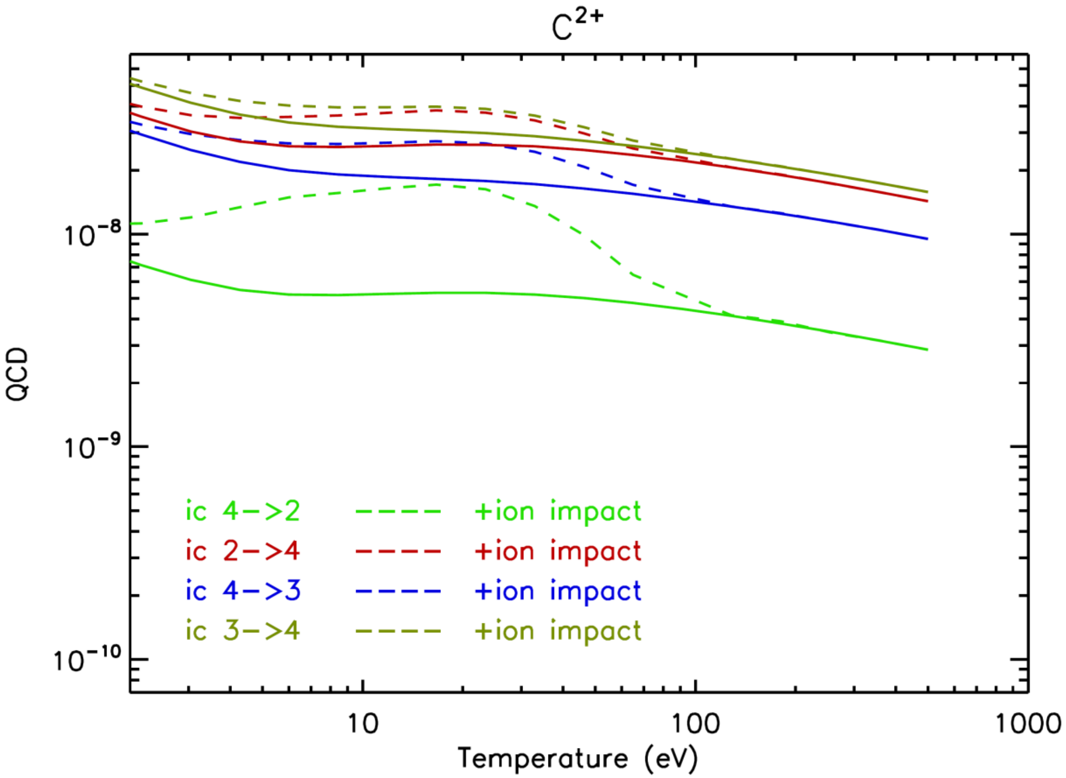
Be-like Carbon example

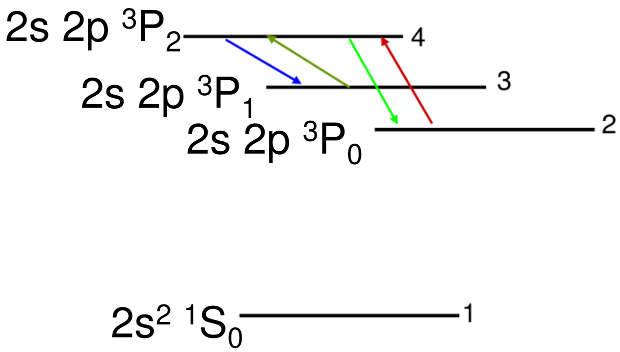




Ion impact contribution on Q_{CD}

Only levels within the fine structure are affected significantly by ion impact.





Ion impact and inclusion in ic GCR: approach

- Issue

  Different colliders can contribute to the total metastable cross-coupling coefficient in different plasmas so

  $$\Downarrow$$

  Q_{CD} with ion impact is not suitable for archiving in central ADAS

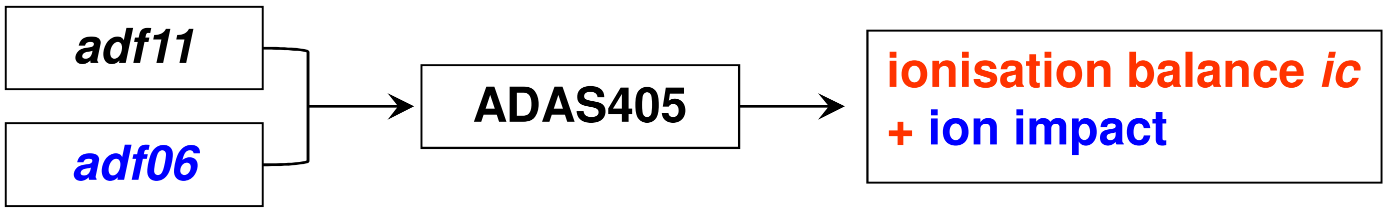
- Method

  Since the alteration due to ion impact is incorporated as an additive term in the Q_{CD} coefficient only, it is convenient and efficient to include its effect in the coefficient on the fly when establishing the ionisation state.

Ion impact and inclusion in ic GCR: status

- First step (*test case*)
  Extend *ls* GCR to intermediate coupling to provide level resolved population distributions and *ic* ionisation balance.

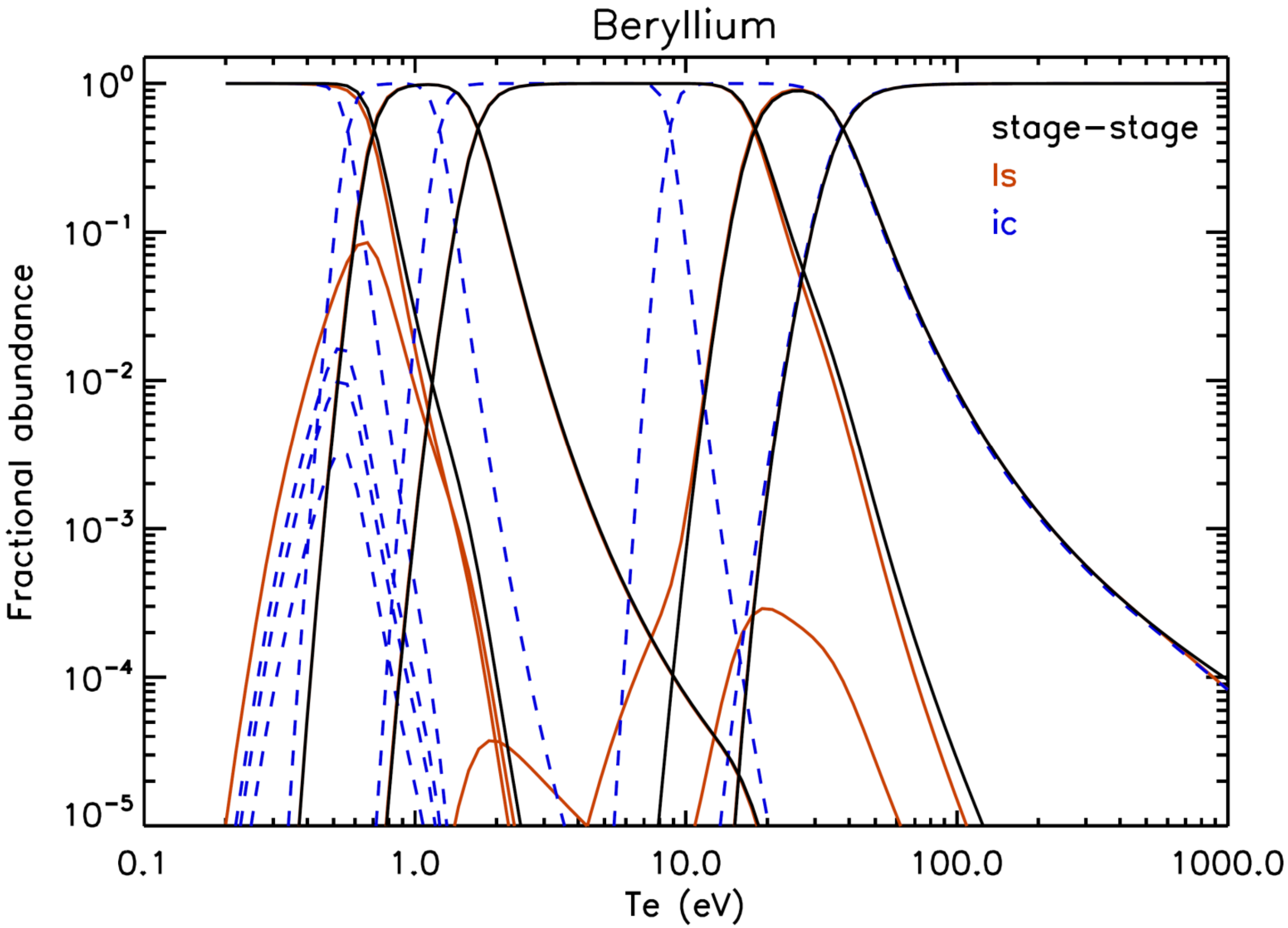
- Second step (*in progress)*
  Add ion impact effect on the fly at the ionisation balance calculation stage.



- Third step (*in progress)*
  Perform contraction into appropriate superstages. This is required moving towards medium weight species when the number of *ic* stages becomes large (e.g. for Si from 32 to 55). This permits focus on the key spectroscopic stages.

Level resolved ionisation balance

Beryllium example



Conclusions and future developments

- Finalising *ic* GCR

- Projection
- State selective recombination (*adf48*, *adf09*)
- State selective ionisation (split_adf07.pro)

- Use a mixed resolution *adf11*

- Bundle *ic* → *ls* → stage
- Superstages approach (ADS416)