Collisional ionization for atoms and ions from H to Zn

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Introduction

Every observation of astrophysical objects involving a spectra requires some aspects of atomic data for the interpretation of line fluxes, ratios and ionization state of the emitting plasma. One of the thermal radiation process which determines it, partially, is the collisional ionization (CI). The main goal of this work is to provide a review, extension and update of previous works and be able of fitting the cross sections and ion rate coefficients of all inner/outer shells of ions from H to Zn. The results will be included in SPEX SW, utilized for X-ray spectra modeling, fitting and analysis.

SPEX V3.01.00

SPEX (SPEctral X-ray and UV) is a modelling and analysis sw package optimized for the interpretation of high-resolution cosmic X-ray spectra. Specially suited for fitting spectra of XMM-Newton, Chandra or Suzaku observations and future X-ray missions as Athena.

The main improvements of v3.01.00 are:

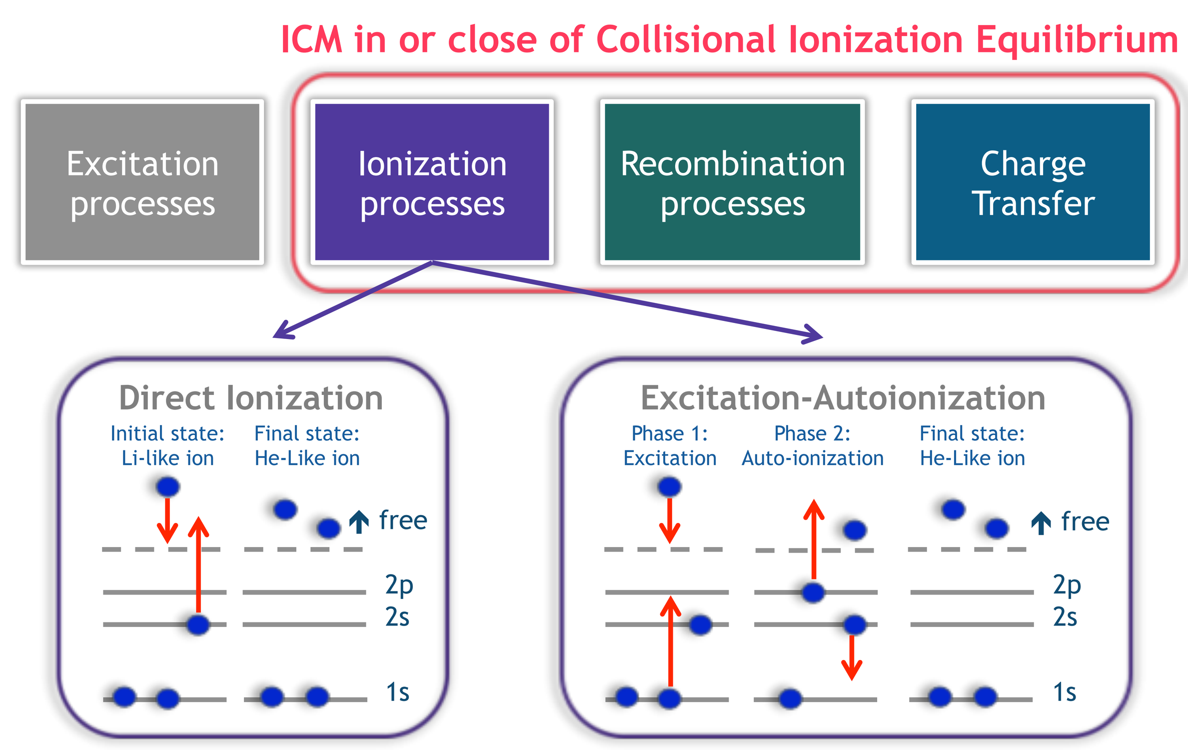
- Fast fitting due to efficient memory and multi-core CPU usage
- Optimization of calculation of all processes
- **New atomic** databases (T. Rassen)
- Improvements of **photo-ionization** model, PION (M. Mehdipour)
- New **charge exchange** model [8]
- Update of **radiative recombination** [9] and **collisional ionization** [10] processes

https://www.sron.nl/spex

Collisional Ionization Process

The main thermal radiation processes can be divided in excitation, ionization, recombination and charge transfer. To calculate the X-ray emission and absorption from plasma the ion concentration is needed, which is obtained solving the equation of ionization balance.

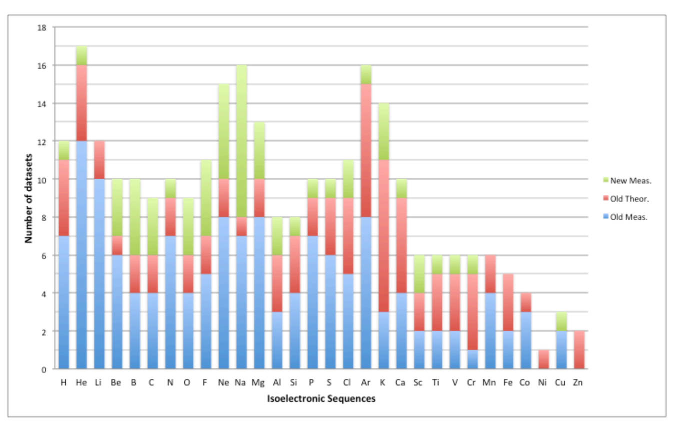
This work is focused on the single collisional ionization process . We have updated the models for the **Direct Ionization (DI)** and **Excitation-Autoionization (EA).**



DI and EA processes. The figure shows DI and EA for Li-like ion with a final state of He-Like ion.

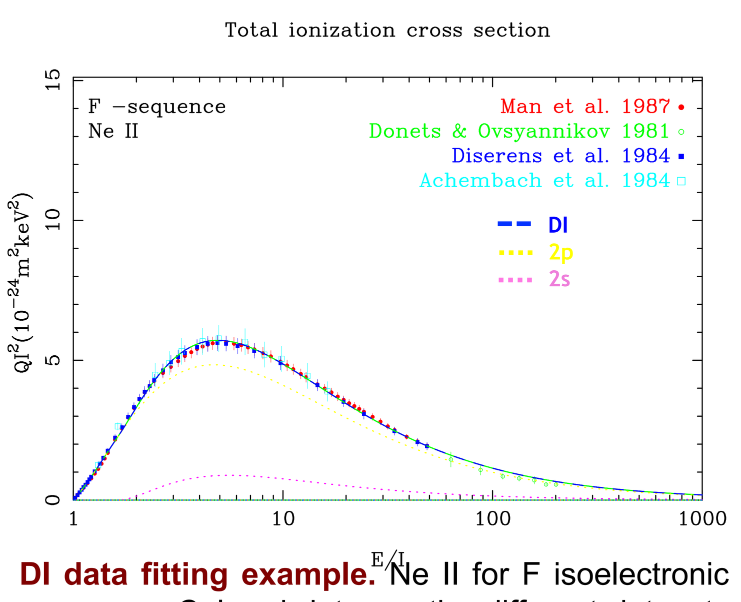
SPEX CI Update Methods

1. Review of the previous and new databases:
   - Arnaud & Raymond 1992 [1]
   - Arnaud & Rorthenflug 1985 [2]
   - Dere 2007 [3]
   - Hahn 2014 [4]
   - IAEA ALADDIN
   - NIFS AMDIS
   - NIST
   - CAMBD



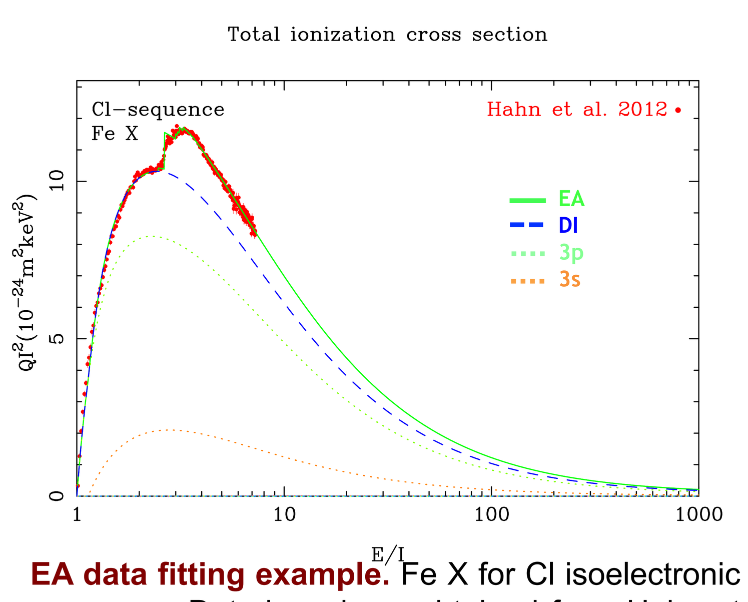
2. DI cross-section fitting per inner shells (extended Younger 1981 [7] formula):
3. EA cross-section fitting (Mewe 1972 [5]) and EA scaled from Sampson&Golden 1981 [6]
4. Rest of elements interpolated or extrapolated
5. Analytical calculation of ion rate coefficients (Arnaud & Rotthenflug 1985 [2])

DI data fitting



DI data fitting example. Ne II for F isoelectronic sequence. Colored dots are the different datasets showed in the figure. Dotted pink line is 2s subshell, dotted orange line 2s subshell, dashed blue line DI contribution.

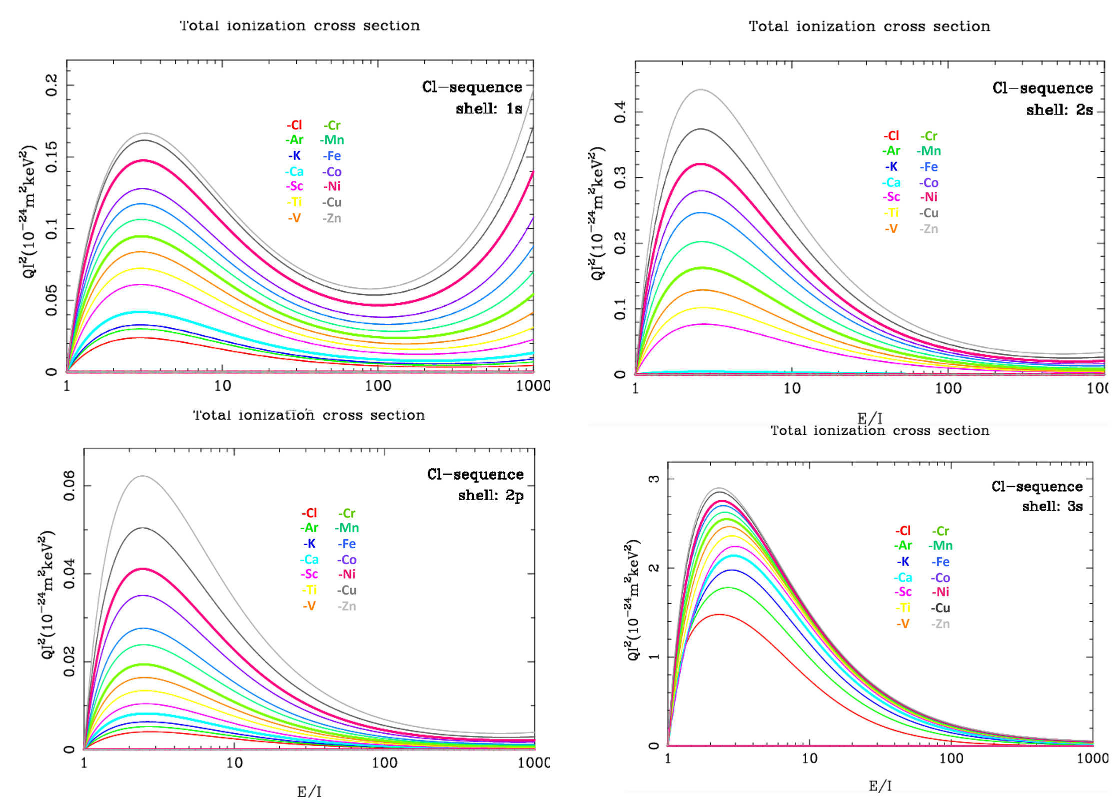
EA data fitting



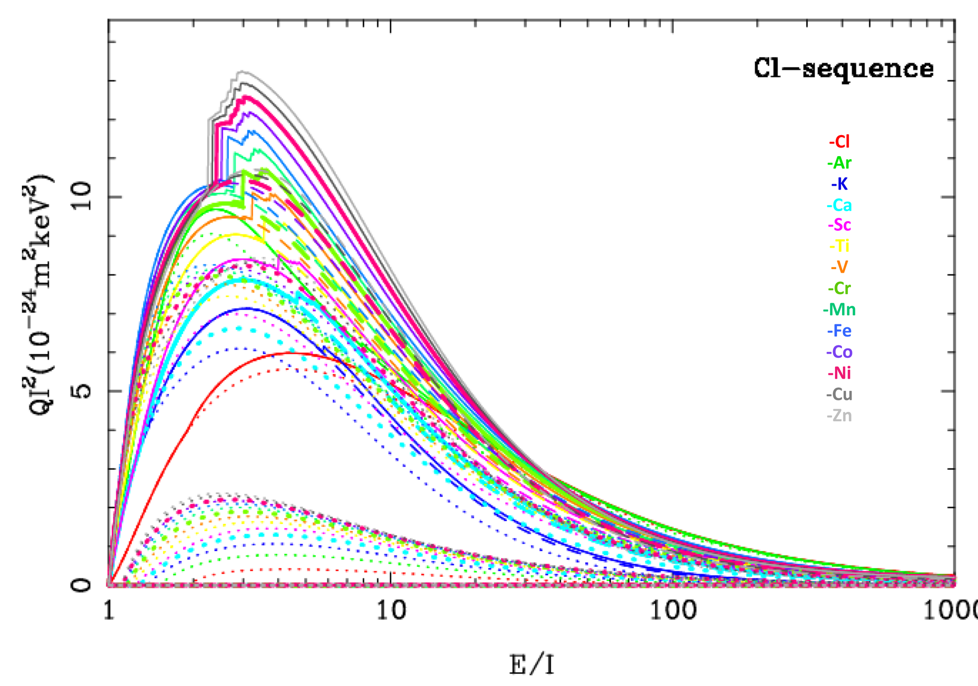
EA data fitting example. Fe X for Cl isoelectronic sequence. Dots in red are obtained from Hahn et al 2012 dataset. Dotted orange line 3s subshell, dotted green line 2p subshell, dashed blue line DI contribution and solid green line EA.

Results

Cl-like isoelectronic sequence (inner and outer shells)



Cl-like inners shells. The figure shows all the inner shells for Cl-like ions. The 1s (upper-left), 2s (upper-right), 2p (lower-left) and 3s (lower right). The sequence elements are represented in different colors.



Cl-like outer shells. Solid line represents the DI+EA component of 3p shell. The upper dotted line is the 3s and the lower dotted line the 2p.

Summary

- Collisional Direct Ionization and Excitation-Autoionization **from H to Zn** processes has been reviewed and updated:

  45 new datasets added.

- **All inner shells** for DI and EA has been modeled:
  - DI cross-section: Extended Younger formula
  - EA cross-section: Mewe formula
  - Extrapolation and interpolation rest of elements

- **Ion rate coefficients** for all inner shells

References

[1] Arnaud & Raymond 1992 ,ApJ. 398, 394
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[3] Dere, 2007, A&A 466, 771
[4] Hahn 2014, JPhCS V488, 012050
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[7] Younger 1981, Quant. Spectr. Radiat.Tran, V27,Nº41
[8] Gu 2016, A&A 588, A52
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