Electron-atom Collisions

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Joint ICTP-IAEA School on Atomic and Molecular Processes in Plasmas

Electron-Atom Collisions

- ✓Processes in Plasma
- ✓Scattering parameter and cross sections (EIE)
- ✓Empirical formulae
- ✓Relativistic distorted wave method
- ✓Example of calculations by FAC and JAC

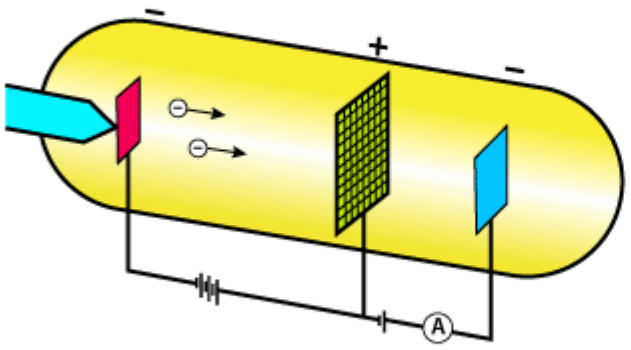
Disclaimer!!

There will be some overlap from yesterday's talk on atomic spectroscopy and tomorrow's lectures on CR modeling.

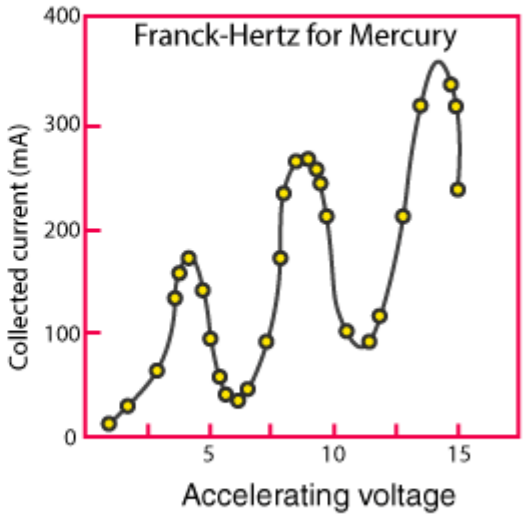
Electron-Atom Collisions

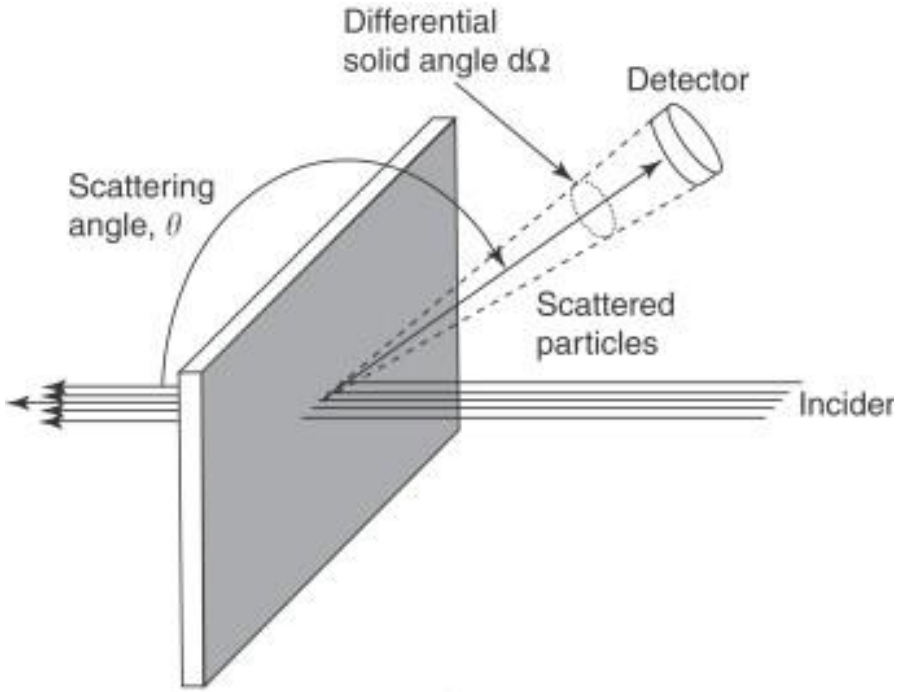
What is the importance?

FRANCK - HERTZ EXPERIMENT

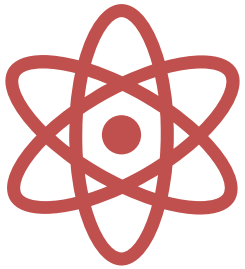


Accelerating apparatus





Atomic processes governing population kinetics in plasma



Collisional Processes

Electron impact excitation

Electron impact de-excitation

Electron impact ionization

Three-body recombination

Autoionization

….

….

Radiative Processes

Photon absorption

Spontaneous radiative decay

Photoionization

Radiative recombination

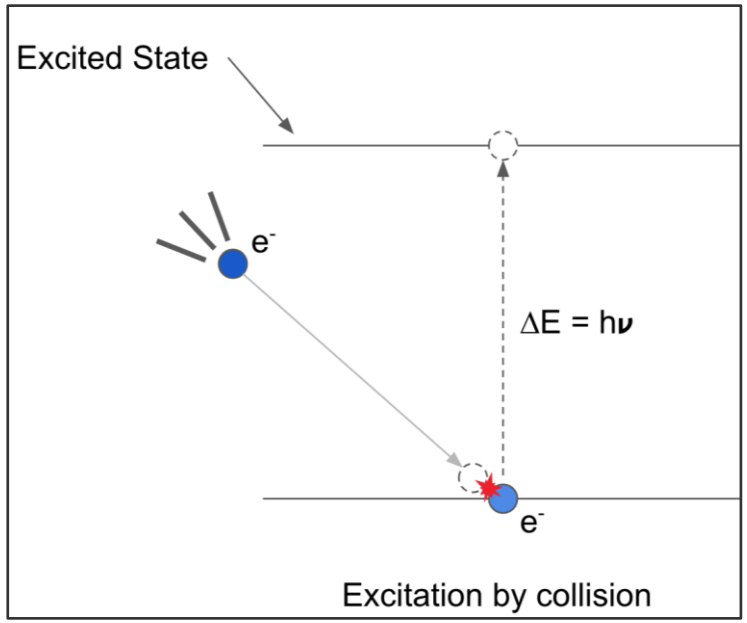
Dielectronic recombination

….

….

Electron-impact excitation ↔ de-excitation (bound–bound)

$$X(i) + e \rightarrow X(f) + e' \qquad\qquad X(f) + e \rightarrow X(i) + e'$$

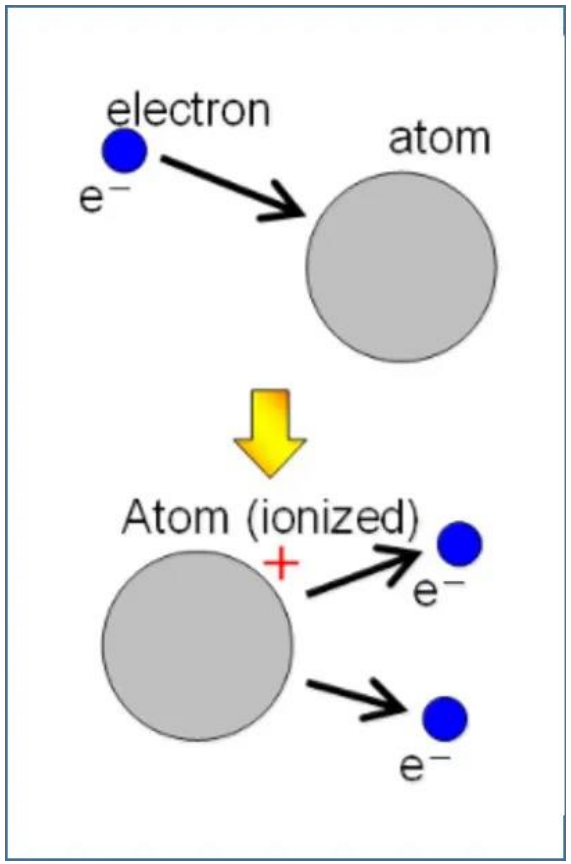


Detailed balance (Maxwellian electrons):

$$k_{fi}^{\text{de-ex}}(T_e) = \frac{g_i}{g_f}\, e^{\Delta E_{fi}/kT_e}\, k_{if}(T_e)$$

Electron-impact ionization ↔ **T**hree-**B**ody **R**ecombination (bound–free)

$$X(i) + e \rightarrow X(f) + \mathrm{e} + \mathrm{e} \qquad X(f) + e + e \rightarrow X(i) + e$$



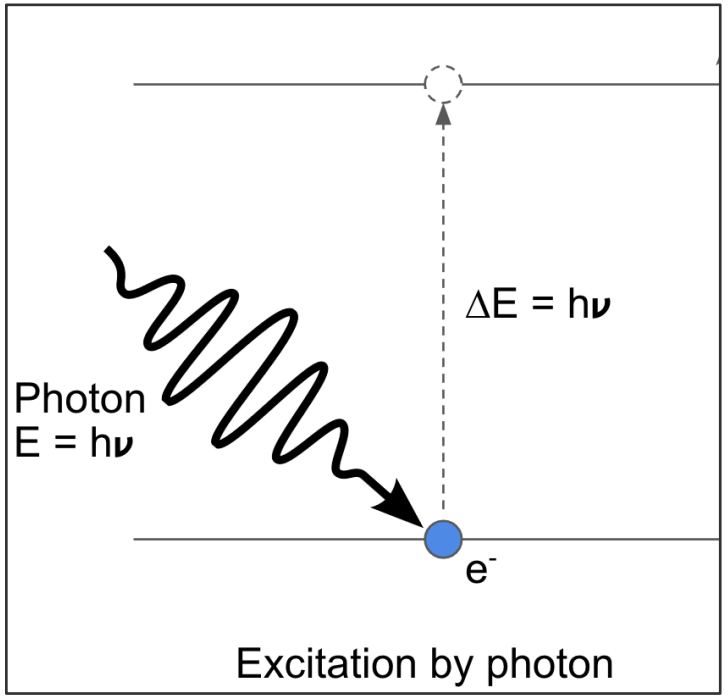
Ionization and TBR are connected through the Saha–Boltzmann relation.

Radiative decay ↔ radiative recombination/photo-excitation

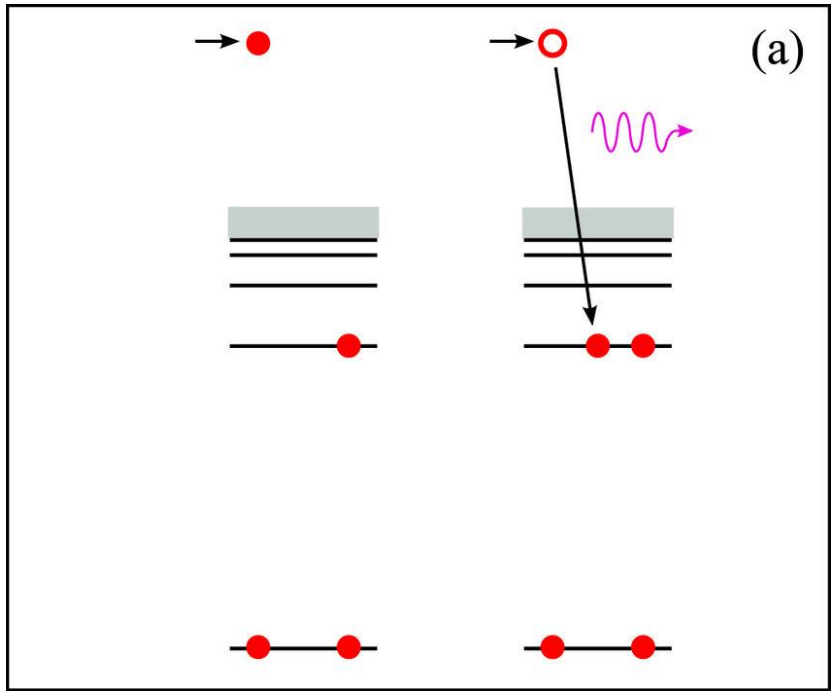
$X(i) \rightarrow X(f) + h\nu (i > f)$

(a) $X(f) + h\nu \rightarrow X(i)$

(b) $X^{+} + e \rightarrow X(i) + h\nu$



Radiative **R**ecombination (RR)



$$g_z \sigma_{ph}(\hbar\omega) = \frac{2mc^2}{\hbar^2\omega^2} g_{z+1} \sigma_{rr}(E)$$

Particle balance equation

Populating upper level 'f' by EIE

Populating upper level 'f' by radiative decay

Populating the next ionic level by TBR

Population into level f – Population out of level f = 0

$$\sum_{\substack{i=1 \\ i\neq f}}^{N} k_{if}^{\mathrm{ex}}(T_e) n_i n_e + \sum_{i>f} A_{if} n_i + n_e n_+ n_e k_{+f}(T_e)$$

$$- \sum_{\substack{i=1 \\ i\neq f}}^{N} k_{fi}^{\mathrm{de-ex}}(T_e) n_f n_e - \sum_{i<f} A_{fi} n_f - n_f n_e k_{f+}(T_e) = 0.$$

depopulating upper level 'f' by EID

depopulating upper level 'f' by radiative decay

depopulating upper level 'f' by EII

Solving the set of linear equations

n_f

Population of f^{th} Level, i.e., number of atoms per unit volume in state f

Line intensity

Theoretical intensity of a line -

$$I_{fi} \propto n_f A_{fi} E_{fi}$$

→ *Difference of energy levels*

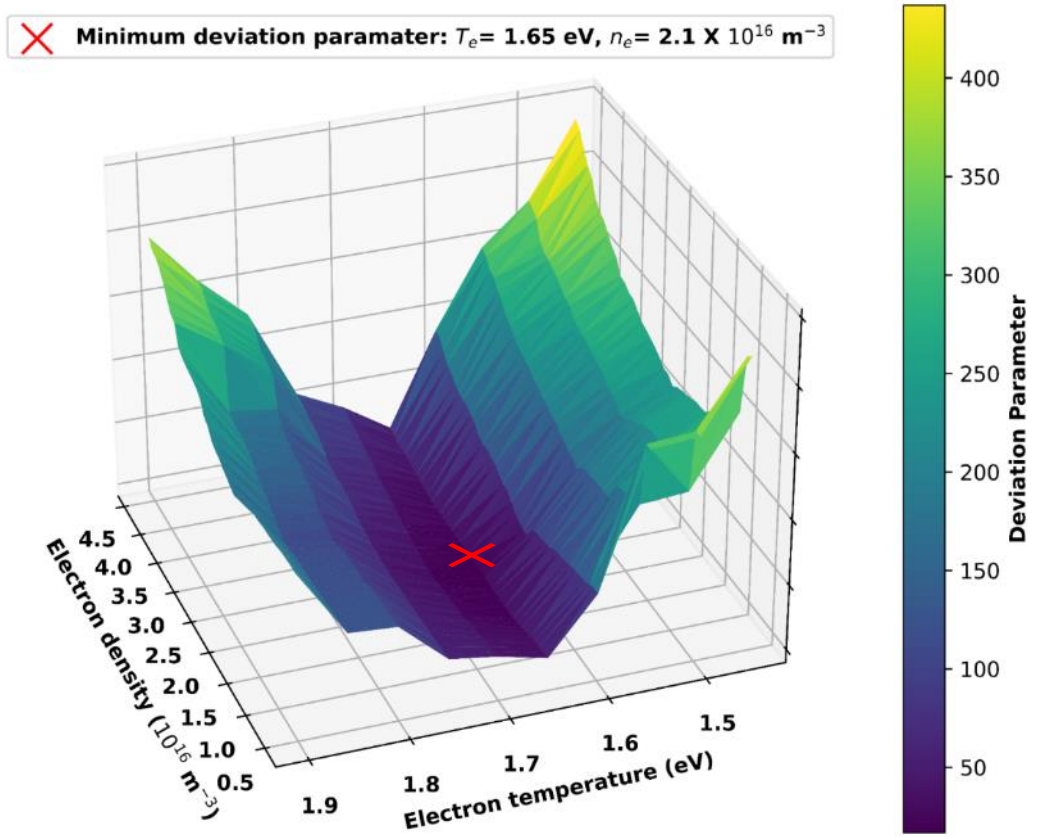
Einstein coefficient of transition

Population of upper level (f^{th})

Normalization of intensity and deviation parameter -

$$I_{f,OES(CRM)}^{normalized} = \frac{I_{f,OES(CRM)}}{\sum_{f=1}^{n} I_{f,OES(CRM)}} \times 100.$$

$$\Delta = \sum_{f=1}^{n} \left(I_{f,OES}^{normalized} - I_{f,CRM}^{normalized} \right)^2.$$



Experiment: (T_e = 1.54 eV and $n_e \sim 10^{16}\ m^{-3}$)

Collision (excitation)

Main *binary* quantity: cross section **σ(E)** [**cm²**]

Effective area for a particular process

$$\sigma(E) = \int |f(E,\theta,\phi)|^2 \, d\Omega$$

f is the scattering amplitude

- Typical values for atomic cross sections
  - $a_0 \sim 5 \cdot 10^{-9}$ cm $\Rightarrow \pi a_0^2 \sim 10^{-16}$ cm²
- Collision strength Ω (dimensionless, *on the order of unity*):

$$\sigma_{ij}(E) = \pi a_0^2 \frac{Ry}{g_j E} \Omega_{ij}(E)$$

  - Ratio of cross section to the de Broglie wavelength squared
  - Symmetric w/r to initial and final states

Atomic Units

h/2π = hbar = 1
mass = mass of electron = m_e = 1
charge = charge of proton= e = 1
length = bohr radius = a_0 = 1

energy = e^2/a_0 = 1 hartree = 27.211385 eV = 627.509 kcal·mol^{-1}=4.3597×10^{-18} J

From cross sections to rates

Rate coefficients for an arbitrary energy distribution function

$$\langle \sigma v \rangle = \int_{E_{min}}^{E_{max}} \sigma(E) v(E) f(E) dE \xrightarrow{Maxw} \left(\frac{8}{\pi m T^3} \right)^{1/2} \int_{\Delta E}^{\infty} E \cdot \sigma(E) \cdot e^{-E/T} dE$$

Effective collision strength:

$$\gamma(T_e) = \frac{1}{T_e} \int \Omega(E) \exp\left(-\frac{E}{T_e} \right) dE$$

Types of transitions for excitation

- Optically(dipole)-allowed
  - $P \cdot P' = -1$ (different parity)
  - $|\Delta l| = 1$
  - $\Delta S = 0, \Delta J = 0, \pm 1$
  - $\sigma(E \rightarrow \infty) \sim \ln(E)/E$
- Optically(dipole)-forbidden
  - $\Delta S = 0$
  - $\sigma(E \rightarrow \infty) \sim 1/E$
- Spin-forbidden (EXCHANGE!)
  - $\Delta S \neq 0$
  - $\sigma(E \rightarrow \infty) \sim 1/E^3$

Examples in He I:

$1s^2\ {}^1S_0 \rightarrow 1s2p\ {}^1P_1$
$1s2p\ {}^3P_1 \rightarrow 1s4d\ {}^3D_2$

$1s2s\ {}^1S_0 \rightarrow 1s3s\ {}^1S_0$
$1s2s\ {}^3S_0 \rightarrow 1s4d\ {}^3D_1$

$1s^2\ {}^1S_0 \rightarrow 1s2p\ {}^3P_1$
$1s2p\ {}^3P_1 \rightarrow 1s4d\ {}^1D_2$

General order
optically allowed > optically forbidden > spin forbidden

van Regemorter-Seaton-Bethe formula

- Optically-allowed excitations

$X \equiv E/\Delta E_{ij}$

$$\sigma_{ij}(E) = \pi a_0^2 \frac{8\pi}{\sqrt{3}} \left(\frac{Ry}{\Delta E_{ij}}\right)^2 \frac{g(X)}{X} f_{ij}$$

Gaunt factor

oscillator strength

$$X \to \infty: \; g(X) \approx \frac{\sqrt{3}}{2\pi} \ln(X) \qquad \sigma(E) \approx \frac{6.51 \cdot 10^{-14}}{(\Delta E[eV])^2} \frac{\ln(X)}{X} f_{ij} \quad [cm^{-2}]$$

"*Recommended*" Gaunt factors:

Atoms:

$$g(\Delta n = 0, X) = \left(0.33 - \frac{0.3}{X} + \frac{0.08}{X^2}\right) \ln(X)$$

$$g(\Delta n \neq 0, X) = \left(\frac{\sqrt{3}}{2\pi} - \frac{0.18}{X}\right) \ln(X)$$

Ions:

$$g(\Delta n = 0, X) = \left(1 - \frac{1}{Z}\right)\left(0.7 + \frac{1}{n}\right)\left[0.6 + \frac{\sqrt{3}}{2\pi} \ln(X)\right]$$

$$g(\Delta n \neq 0, X) = 0.2 (X < 2), \; \frac{\sqrt{3}}{2\pi} \ln(X) \;\; for \; X \geq 2$$

Scattering amplitude and cross section

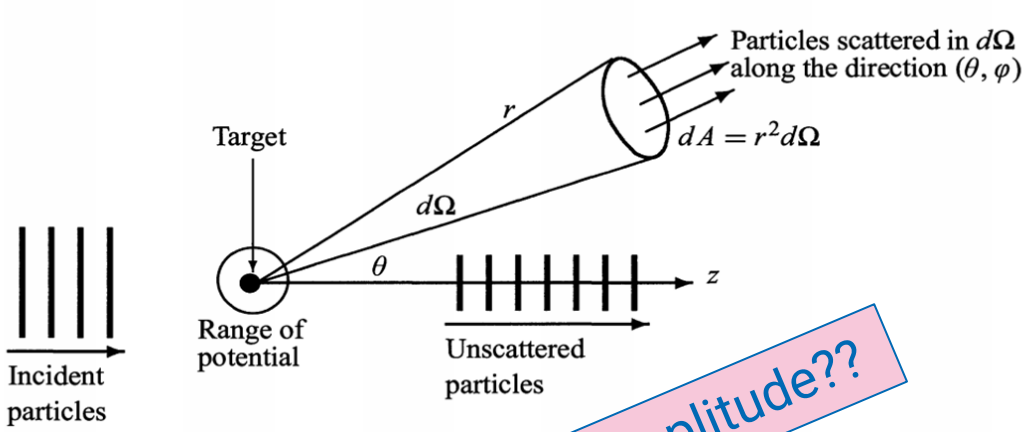
- After scattering the total wave consists of a superposition of incident plane wave and the scattered wave .

$$\psi(\vec{r}) = \phi_{inc}(\vec{r}) + \phi_{sc}(\vec{r}) \; A\left[\exp(i\vec{k}_0.\vec{r}) + f(\theta,\varphi)\frac{\exp(i\vec{k}.\vec{r})}{r}\right]$$

- The incident and scattered flux densities:

$$\vec{J}_{inc} = \frac{i\hbar}{2\mu}\left(\phi_{inc}\vec{\nabla}\phi^*_{inc} - \phi^*_{inc}\vec{\nabla}\phi_{inc}\right) = |A|^2\frac{\hbar k_0}{\mu},$$

$$\vec{J}_{sc} = \frac{i\hbar}{2\mu}(\phi_{sc}\vec{\nabla}\phi^*_{sc} - \phi^*_{sc}\vec{\nabla}\phi^*_{sc}) = |A|^2\frac{\hbar k}{\mu r^2}|f(\theta,\varphi)|^2.$$



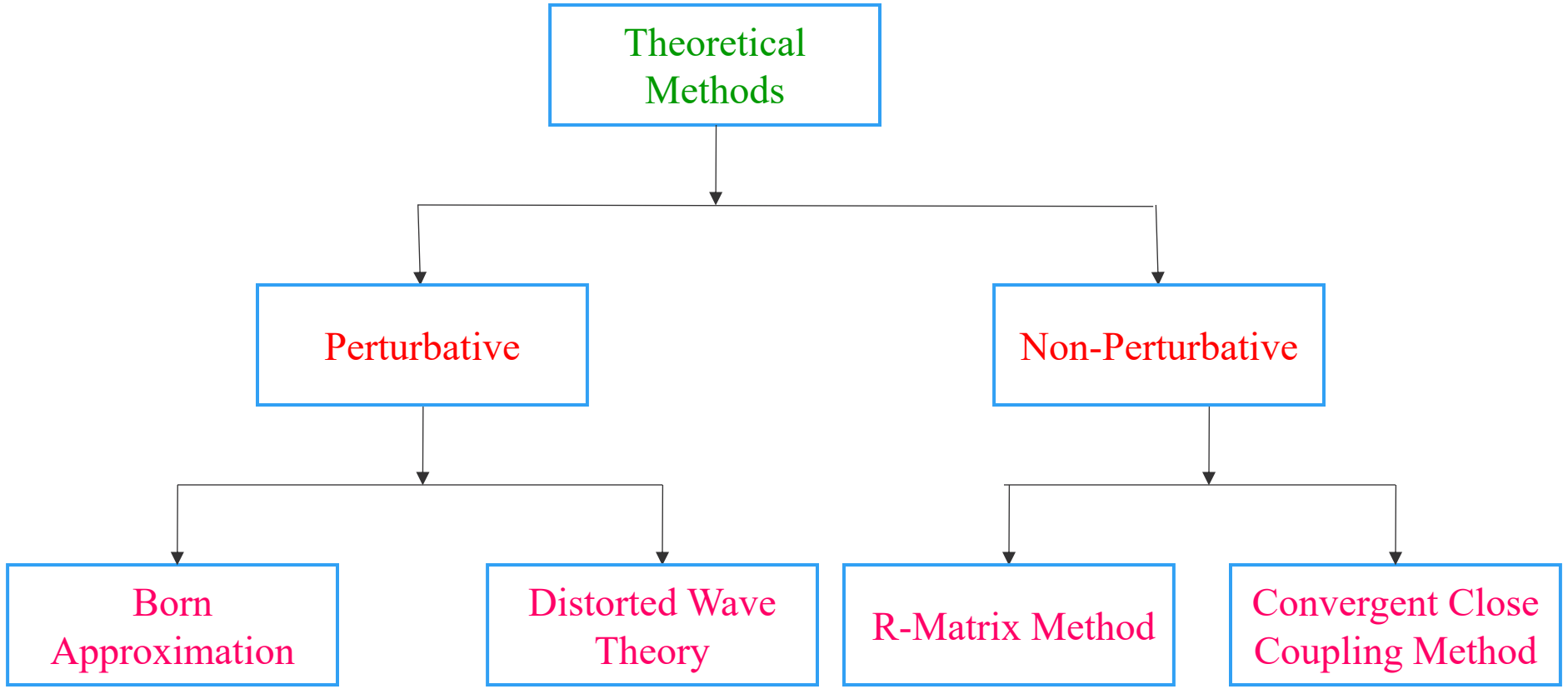
How to obtain scattering amplitude??

- The Differential cross section then will be-

$$\frac{d\sigma}{d\Omega} = \frac{1}{J_{inc}}\frac{dN}{d\Omega} = \frac{k}{k_0}|f(\theta,\varphi)|^2$$

- Integrated cross sections

$$\sigma = \int \frac{d\sigma}{d\Omega}d\Omega = \int_0^{\pi}\sin\theta\, d\theta \int_0^{2\pi}\frac{d\sigma(\theta,\varphi)}{d\Omega}d\varphi.$$



These methods have been extensively explored in both relativistic and non-relativistic forms

Electron impact excitation (EIE) of atoms/ions

Methodology

Relativistic distorted wave (RDW) T − matrix

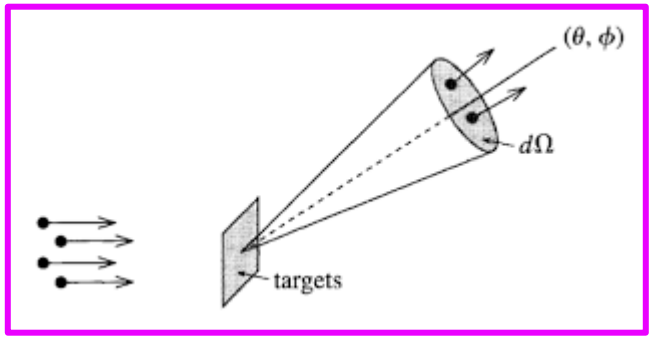
$$\boldsymbol{T_{a\to b}} = \left\langle \Phi_b(\mathbf{1},\mathbf{2},\dots,\boldsymbol{N}) F_b^{DW-}(\boldsymbol{k_b},\boldsymbol{N}+\mathbf{1}) \middle| V_{in} - U_d(N+1) \middle| \boldsymbol{A}\, \Phi_a(\mathbf{1},\mathbf{2},\dots,\boldsymbol{N}) F_a^{DW+}(\boldsymbol{k_a},\boldsymbol{N}+\mathbf{1}) \right\rangle$$

$\Psi_{a(b)}$ Target atom wave function before(after) scattering

V_{in} Interaction potential

U_d Distortion potential

$F_{a(b)}^{DW+(-)}$ Projectile electron distorted wave function



$$V_{in}(r_i,r_j) = V^{Coulomb} + V^{Breit} = -\frac{Z}{r_{N+1}} + \sum_{i<j}\left(\frac{1}{r_{ij}} - \boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j\frac{1}{r_{ij}} + \frac{1}{2}\,(\boldsymbol{\alpha}_i\cdot\boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_j\cdot\boldsymbol{\nabla}_j)r_{ij}\right)$$

Collision Parameters of interest

Differential and integrated cross sections

Excitation rate coefficients

Fitting parameters for cross sections

Sahoo et al, *Eur. Phys. J. Plus (2024) 139:986*

This T-matrix can be decomposed into it's direct and exchange components

$$T_{a\to b} = T^{d}_{a\to b} + T^{ex}_{a\to b}$$

with

$$T^{d}_{a\to b} = \left\langle \Phi_b(1,2,...,N) F_b^{DW-}(k_b, N+1) \middle| V - U_b(N+1) \middle| \times \Phi_a(1,2,...,N) F_a^{DW+}(k_a, N+1) \right\rangle,$$

and

$$T^{ex}_{a\to b} = \left\langle \Phi_b(1,2,...,N) F_b^{DW-}(k_b, N+1) \middle| V - U_b(N+1) \middle| \times \sum_{j=1}^{N} (-1)^{N+1-j} \Phi_a(-j) F_a^{DW+}(k_a, j) \right.$$

where $\Phi_a(-j)$ denotes atomic wave function with coordinate j absent and coordinate N+1 included

Exchange T-matrix can be written as the sum of three exchange terms

$$T^{ex}_{a\to b} = T^{ex1}_{a\to b} + T^{ex2}_{a\to b} + T^{ex3}_{a\to b}$$

where

$$T^{ex1}_{a\to b} = -N\left\langle \Phi_b(1,2,\ldots,N)F_b^{DW-}(k_b,N+1)\left|-\frac{Z}{r_{N+1}} - U_b(N+1)\right|\Phi_a(1,2,\ldots,N-1,N+1)F_a^{DW+}(k_a,N)\right\rangle,$$

$$T^{ex2}_{a\to b} = -N\left\langle \Phi_b(1,2,\ldots,N)F_b^{DW-}(k_b,N+1)\left|\frac{1}{|r_{N+1}-r_N|}\right|\Phi_a(1,2,\ldots,N-1,N+1)F_a^{DW+}(k_a,N)\right\rangle,$$

$$T^{ex3}_{a\to b} = -N\left\langle \Phi_b(1,2,\ldots,N)F_b^{DW-}(k_b,N+1)\left|\sum_{j=1}^{N}\frac{1}{|r_{N+1}-r_j|}\right|\Phi_a(1,2,\ldots,N-1,N+1)F_a^{DW+}(k_a,N)\right\rangle,$$

Computation of T-matrix

First few energy levels of Sn I (Z = 50, [Kr] $4d^{10}\ 5s^2\ 5p^2$)

Configuration	Term	J	Level (eV)
$5s^25p^2$	^3P	0	0.0000000
		1	0.2097572
		2	0.4249773
$5s^25p^2$	^1D	2	1.0678703
$5s^25p^2$	^1S	0	2.1278787
$5s^25p6s$	$^3P^\circ$	0	4.2949066
		1	4.32881927
		2	4.78937023
$5s^25p6s$	$^1P^\circ$	1	4.86725425

NIST ASD

How these atomic states are represented in multi-configuration Dirac-Hartree-Fock approximation

In the relativistic j-j coupling scheme, the ground state all shells except s are broken into two subshells

$\bar{p}$ represents an electron with ℓ = 1 and j =1/2

p represents an electron with ℓ = 1 and j =3/2

Outershell configuration $5p^2$

Five fine-structure levels ($^1S_0$, $^1D_2$, $^3P_{0,1,2}$)

In relativistic notations:

Ground state configuration $5p^2$:

$5\bar{p}^2\ (J = 0, 1),$

$5p^2 (J = 0, 2),$

$5\bar{p}5\mathrm{p}\ (\mathrm{J} = 2)$

Excited state Configuration $5p6p$:

$5\bar{p}6\bar{p}\ (J = 0, 1),$

$5\bar{p}6\mathrm{p}\ (\mathrm{J} = 1, 2),$

$5\mathrm{p}6\bar{p}\ (J = 1, 2),$

$5p6p\ (J = 0, 1, 2, 3)$

J	No of levels
0	4
1	5
2	5
3	1

$$^3P_0,\ ^1S_0,: a_1 5\bar{p}^2 + a_2 5\bar{p}6\bar{p} + a_3 5p^2 + a_4 5p6p$$

$$^3P_1: a_1 5\bar{p}^2 + a_2 5\bar{p}6\bar{p} + a_3 5\bar{p}6p + a_4 5p6\bar{p} + a_5 5p6p$$

$$^3P_2,\ ^1D_2: a_1 5\bar{p}5p + a_2 5\bar{p}6p + a_3 5p^2 + a_4 5p6\bar{p} + a_5 5p6p$$

J	No of levels
0	4
1	5
2	5
3	1

Initial states	a_1	a_2	a_3	a_4	a_5
$^3P_0$	0.8900	0.3289	-0.4550	-0.0283	0
$^3P_1$	0.9998	$2.67\text{x}10^{-5}$	0.0146	0.0166	0.0013
$^3P_2$	0.7455	0.0029	0.6659	-0.0074	0.0261
$^1D_2$	-0.6659	0.0248	0.7455	-0.0123	-0.0063
$^1S_0$	0.4504	-0.0761	0.8856	-0.0833	0

a_i's are calculated using GRASP2018

Excited state representation:

$5p6s$:

$5\bar{p}6s\ (J = 0,1),$

$5p6s\ (J = 1,2)$

$5p5\mathrm{d}$:

$5\bar{p}5\bar{\mathrm{d}}(J = 1,2),$

$5p5\bar{\mathrm{d}}(J = 0,1,2,3),$

$5\bar{p}5d\ (J = 2,3),$

$5p5d\ (J = 1,2,3,4)$

J	No of levels
0	2
1	5
2	5

$^3P_0 : b_1 5\bar{p}6s + b_2 5p5\bar{d}$

$^3P_1,\ ^1P_1 : b_1 5\bar{p}\ 5\bar{d} + b_2 5\bar{p}6s + b_3 5p5\bar{d} + b_4 5p5d + b_5 5p6s$

$^3P_2, : b_1 5\bar{p}\ 5\bar{d} + b_2 5\bar{p}\ 5d + b_3 5p5\bar{d} + b_4 5p5d + b_5 5p6s$

Relativistic distorted wave function

- The relativistic expansion of projectile electron distorted-wave functions

$$F^{DW\pm}_{ch,\mu_{ch}}(k_{ch},r)=\frac{1}{(2\pi)^{3/2}}\sum_{\kappa m} e^{\pm i\eta_\kappa}\, a^{\mu_{ch}}_{ch,\kappa m}(\hat{k}_{ch})\,\frac{1}{r}\begin{pmatrix} f_\kappa(r)\xi_{\kappa m}(\hat{r}) \\ i g_\kappa(r)\xi_{-\kappa m}(\hat{r})\end{pmatrix},$$

$$with$$

$$a^{\mu_{ch}}_{ch,\kappa m}(\hat{k}_{ch})=4\pi i^{i}\left[\frac{E_{ch}+c^2}{2E_{ch}}\right]^{\frac{1}{2}}\sum_{ml}(lm_l 1/2\mu_{ch}|jm)\,Y^*_{lm_l}(\hat{k}_{ch}).$$

The large and small components f_k and g_k of the continuum wave functions satisfy the coupled Dirac equations

$$\left(\frac{d}{dr}+\frac{k}{r}\right)f_\kappa(r)-\frac{1}{c}(c^2-U_{ch}+E_{ch})g_\kappa(r)=0,$$

$$\left(\frac{d}{dr}+\frac{k}{r}\right)f_\kappa(r)-\frac{1}{c}(c^2-U_{ch}+E_{ch})g_\kappa(r)=0$$

These coupled equations can be solved numerically and phase shift can be solved by using boundary conditions.

$$f_\kappa(r) \xrightarrow{r\to\infty} \frac{1}{k_{ch}} \sin\left(k_{ch}r - \frac{l\pi}{2} + \eta_\kappa\right),$$

$$and$$

$$g_k(r) \xrightarrow{r\to\infty} \frac{c}{c^2 + E_{ch}} \cos\left(k_{ch}r - \frac{l\pi}{2} + \eta_\kappa\right)$$

Computation of T – matrices

$$\boldsymbol{T_{a\to b}} = \left\langle \Phi_b(\mathbf{1},\mathbf{2},\dots,\boldsymbol{N}) F_b^{DW-}(\boldsymbol{k_b},\boldsymbol{N}+\mathbf{1}) \middle| V_{in} - U_d(N+1) \middle| \boldsymbol{A}\, \Phi_a(\mathbf{1},\mathbf{2},\dots,\boldsymbol{N}) F_a^{DW+}(\boldsymbol{k_a},\boldsymbol{N}+\mathbf{1}) \right\rangle$$

1. Atomic Structure
2. Distortion potential
3. Projectile electron wavefunction
5. Excitation cross sections
6. Excitation rate coefficients

EIE of Bismuth

❖ Bismuth (Z=83) a heavy element with electronic configuration **[Hg] $6p^3$**.

- Complex outer shell structure with open outer subshells
- No previous theoretical studies for EIE available
- Provides a perfect ground to test the relativistic methods

❖ Marinković *et al.* 2016 performed the EIE from the ground state **$6p^3\ {}^4S_{1/2} \rightarrow 6p^27s\ {}^4P_{1/2}$**

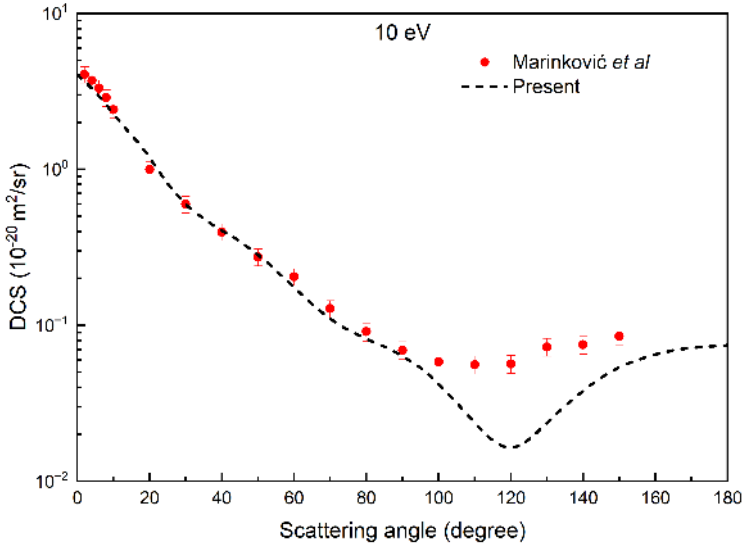
- Reported the differential cross sections in 2 – 150 degree scattering angle range
- Integral cross sections at electron energies 10, 20, 40, 60, 80 and 100 eV.
- Generalized oscillator strengths

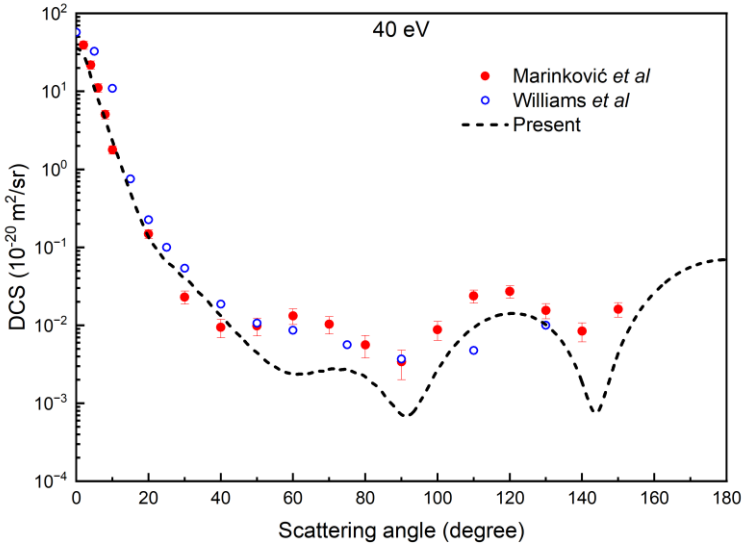
❖ Williams *et al.* 1975 reported the DCS and ICS for 40 eV incident electron energy.

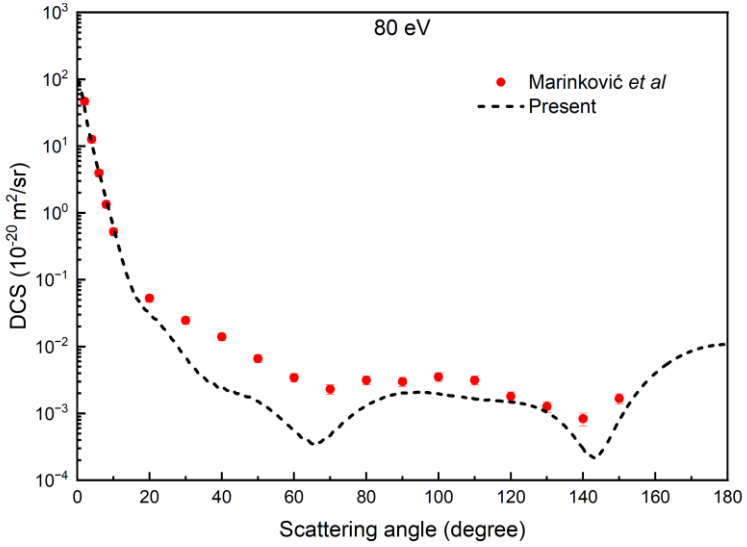
First theoretical investigation of electron impact excitation of bismuth.

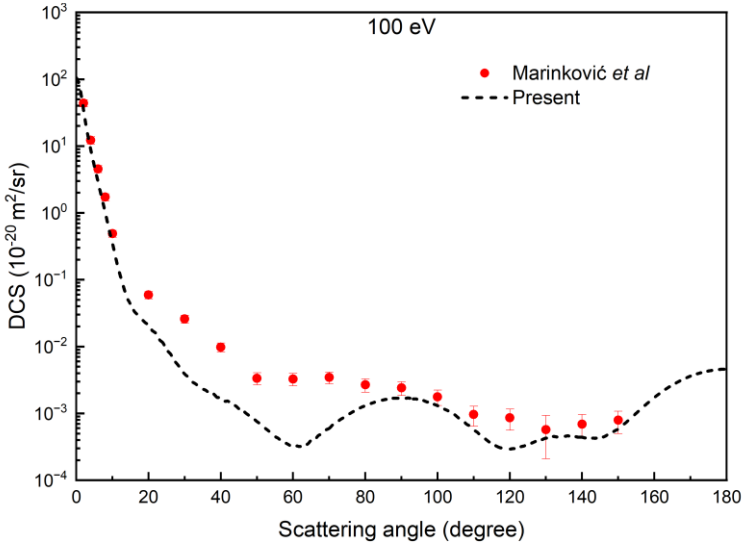
- Marinković, B. P., Predojević, B., Šević, D., & Pejčev, V. Electron impact excitation of the $6p^27s\ {}^4P_{1/2}$ state of bismuth from the ground state. Journal of Physics B: Atomic, Molecular and Optical Physics, 49(23), 235203 (2016).
- Williams, W., Trajmar, S., & Bozinis, D. G. Elastic and inelastic scattering of 40 eV electrons from atomic and molecular bismuth. Journal of Physics B: Atomic and Molecular Physics, 8(6), L96 (1975).

DCS Results



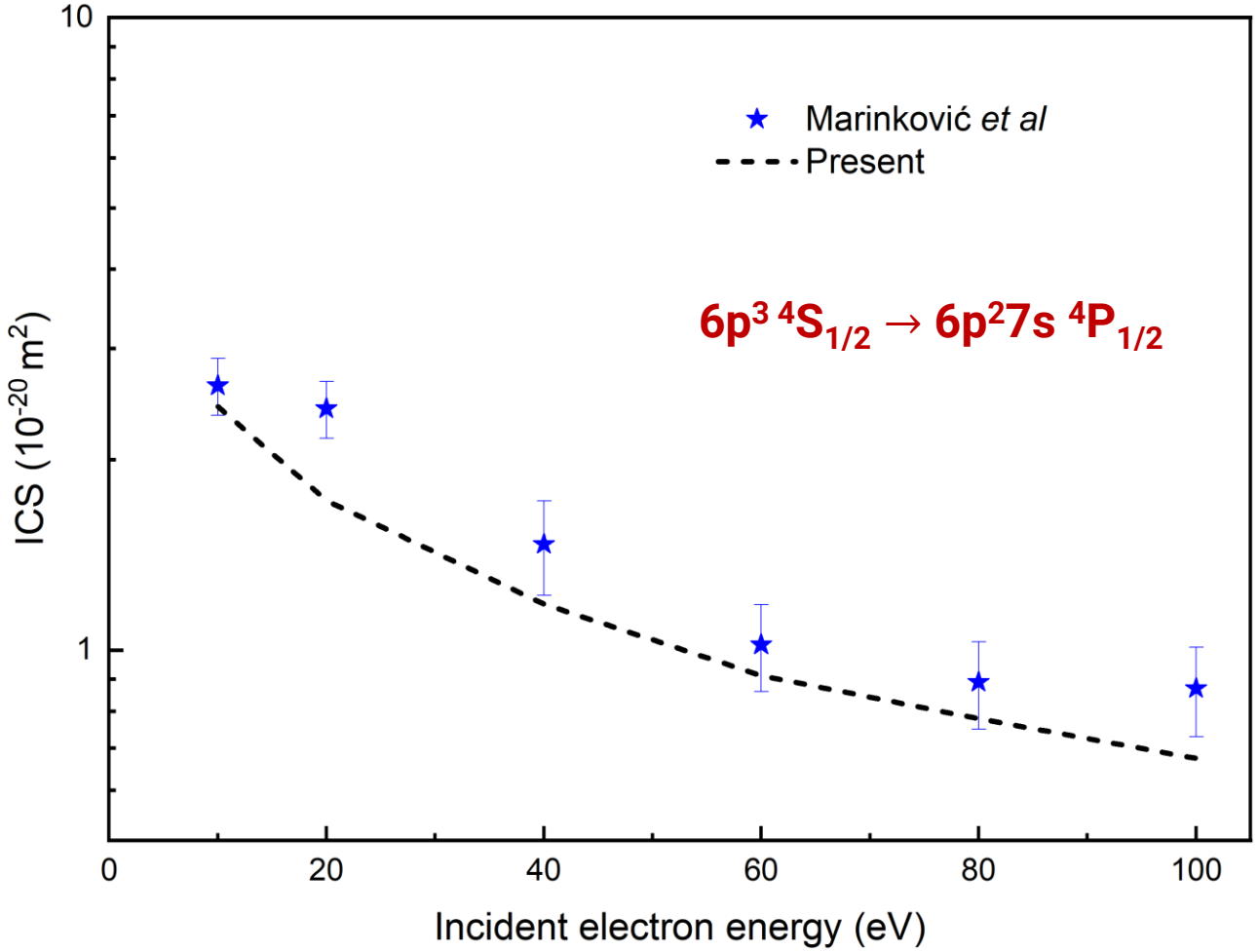






- Marinković, B. P., Predojević, B., Šević, D., & Pejčev, V. *Journal of Physics B: Atomic, Molecular and Optical Physics*, *49*(23), 235203 (2016).

ICS Results

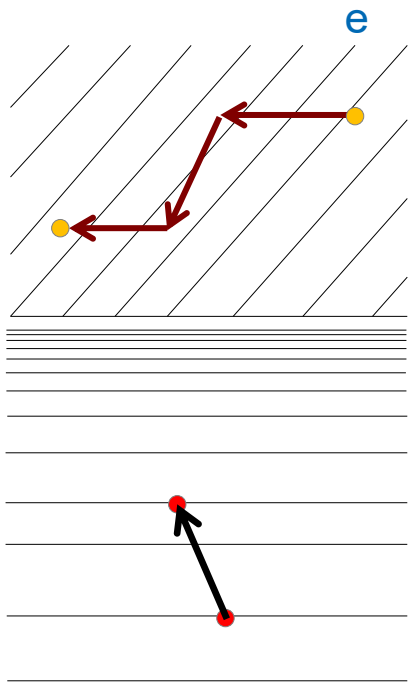


Experiment: Marinković, B. P., Predojević, B., Sević, D., & Pejčev, V. (2016). *Journal of Physics B: Atomic, Molecular and Optical Physics*, *49*(23), 235203.

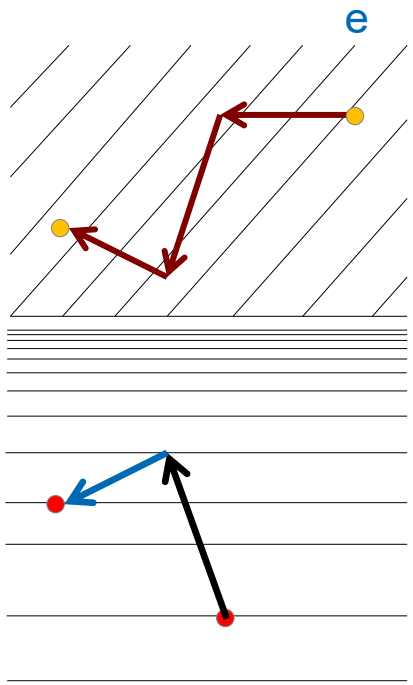
Sahoo, Sharma. Physica Scripta 99 (9), 095410, 2024

Drawbacks

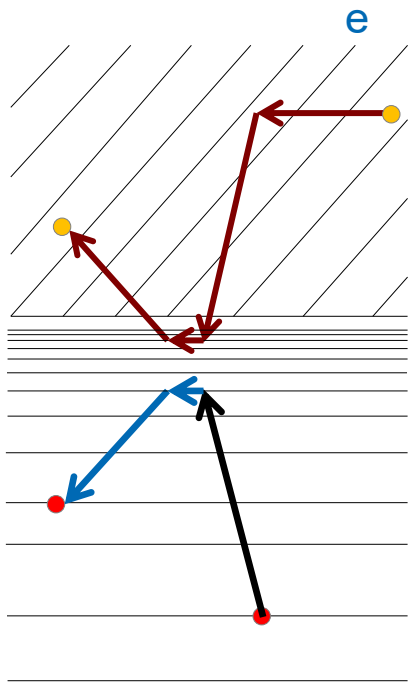
Resonances in excitation



Direct excitation

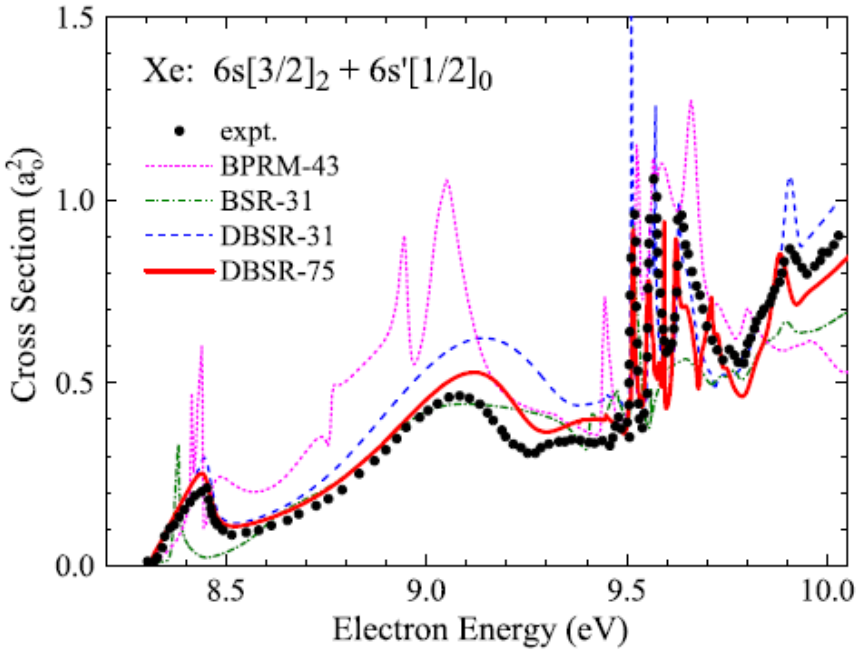


Intermediate states

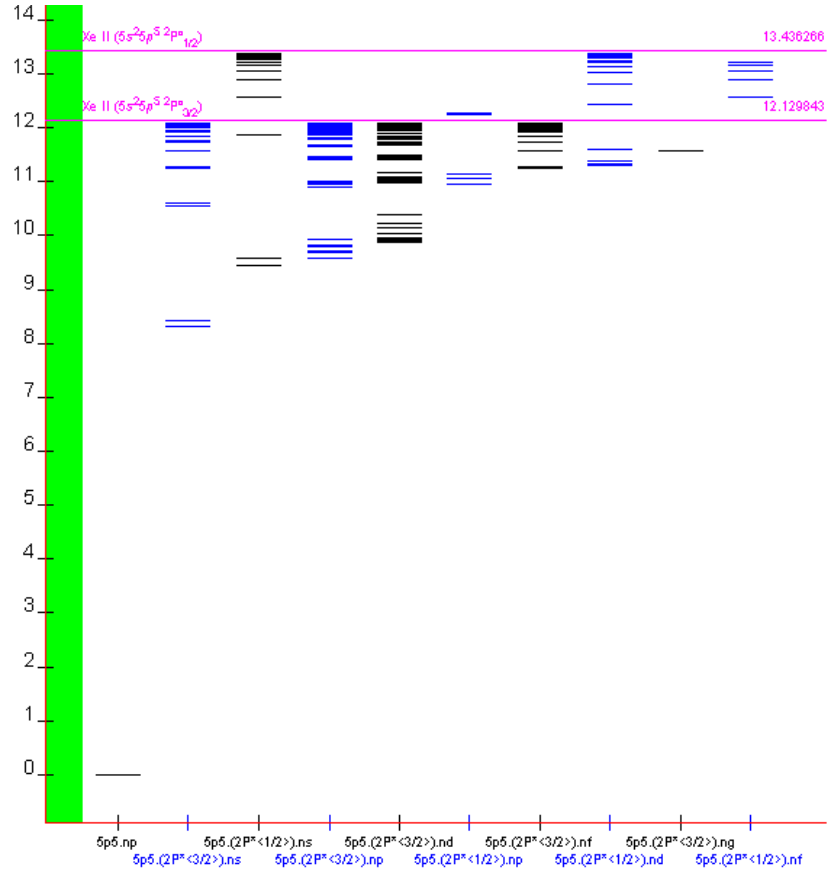


Intermediate AI states

Experiment vs theory



Zatsarinny and Bartschat, 2010



NIST ASD Grotrian Diagram

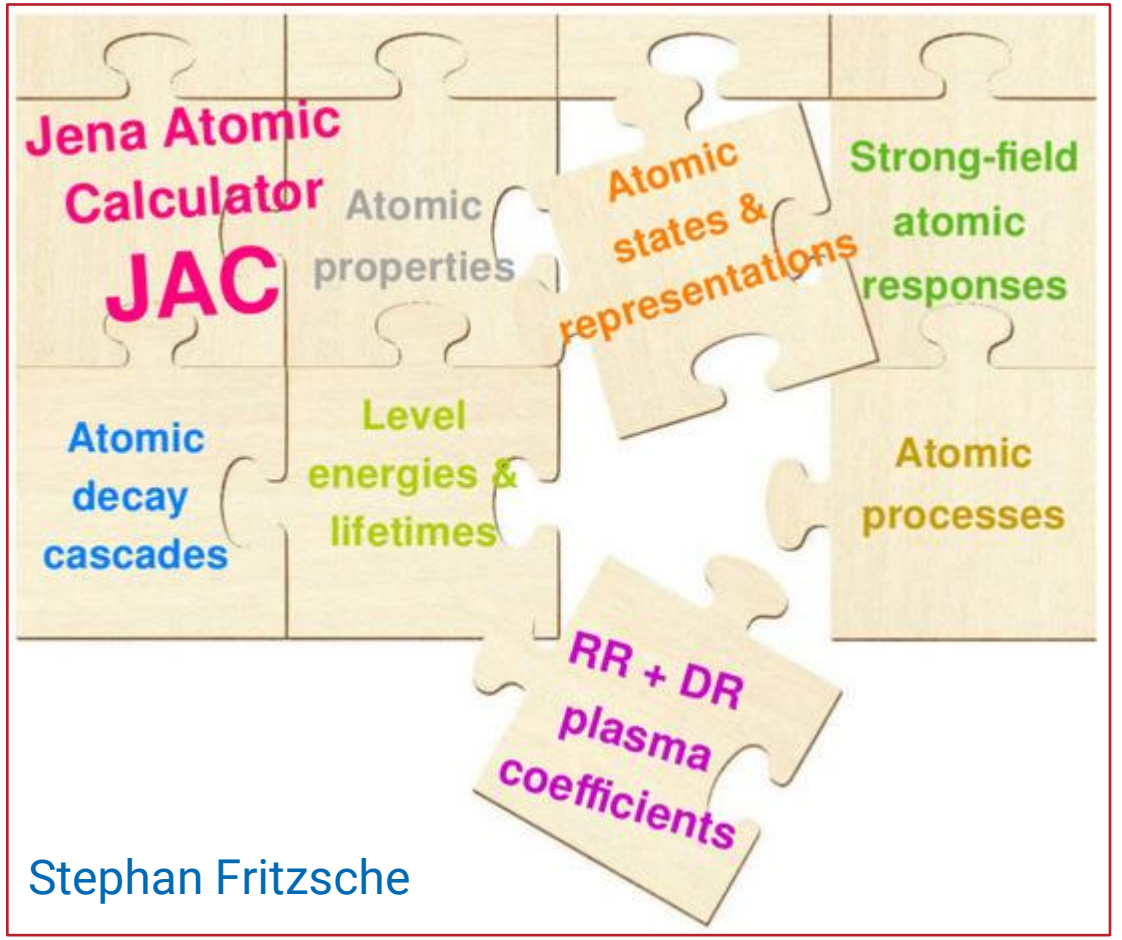
Available Codes for Atomic Collision Calculations

flexible-atomic-code/**fac**

FAC - Flexible Atomic Code by Ming Feng Gu

5 Contributors · 58 Issues · 95 Stars · 59 Forks

M F Gu



Stephan Fritzsche

Atomic processes implemented in FAC

- Structure: solving Dirac equation –> energy levels (QED corrections)
- Radiative transition.
- Electron impact excitation.
- Electron impact ionization.
- Photoionization, radiative recombination.
- Autoionization, dielectronic capture.
- A simple collisional radiative model for spectral modeling
- Excitation and ionization between magnetic sublevels, linear polarization in EBITs.
- External E&B fields.
- Screening potential of plasma electrons.
- 2nd order MBPT + CI
- Dirac R-Matrix for excitation
- Electron impact Stark broadening.

Download and Installation

- https://github.com/flexible-atomic-code/fac
- git clone https://github.com/flexible-atomic-code/fac
- git pull
- Requires python, c, f77 compilers (gcc and gfortran work fine)
- ./configure --with-mpi=omp --prefix=install_dir
- make
- make install
- make pfac
- make install-pfac
- python setup.py install --prefix=install_dir

Electronic configurations & Angular coupling

- Non-relativistic subshells, 1s, 2s, 2p, 3d, 4f, etc
- Relativisitic subshells, 1[s+], 2[p-], 3[d+], “-”: j=l-1/2, “+”: j=l+1/2
- For large orbital angular momentum, 30[26], n=30, l=26
- Configurations, ‘1s2 2s2 2p4’, occupations directly follow subshells
- “*” can denote any orbital angular momenta. ‘3*1’ expands to 3s1, 3p1, 3d1 configurations.
- Restriction on electron occupation, ‘3*10;3d<3’, all possible ways of distributing 10 electrons in 3s, 3p, 3d subshells, with no more than 3 electrons in 3d. Multiple conditions separated by “;” with logical and. ‘3*10;3d>1;3d<4’, 3d must have 2 or 3 electrons.
- Angular momentum coupling, 2p+3(3)3 3s+1(1)4

Example of Ne-like Fe

```
fac.SetAtom('Fe')
# 1s shell is closed
fac.Closed('1s')
fac.Config('2*8', group = 'n2')
fac.Config('2*7 3*1', group = 'n3')

# Self-consistent iteration for optimized central potential
fac.ConfigEnergy(0)
fac.OptimizeRadial('n2')
fac.ConfigEnergy(1)
fac.Structure('ne.lev.b')
fac.MemENTable('ne.lev.b')
fac.PrintTable('ne.lev.b', 'ne.lev', 1)

fac.CETable('ne.ce.b', ['n2'], ['n3'])
fac.PrintTable('ne.ce.b', 'ne.ce', 1)
```

Ne-like Fe cont…

```
# version numbers
FAC 1.0.4
# binary order used in the binary file
Endian = 0
# time stamp when the file was created.
TSess = 1020438482

 # database type
 Type = 1
 # this file is in verbose form
 Verbose = 1
 # atomic symbol and atomic number
 Fe Z = 26.0
 # number of data blocks in this file
 NBlocks = 1
 # the index and the absolute energy of the ground state
 E0 = 0, -3.12494784E+04

 # data block begins
 # number of electron for the states in this block
 NELE = 10
 # number of levels in this block
 NLEV = 37
   ILEV  IBASE    ENERGY       P   VNL 2J
```

Ne-like Fe cont…

```
......
NELE = 10
NLEV = 37
  ILEV  IBASE    ENERGY        P   VNL 2J
     0     -1  0.00000000E+00 0   201   0 1*2 2*8        2p6          2p+4(0)0
     1     -1  7.23817529E+02 1   300   4 1*2 2*7 3*1    2p5 3s1      2p+3(3)3 3s+1(1)4
     2     -1  7.25866864E+02 1   300   2 1*2 2*7 3*1    2p5 3s1      2p+3(3)3 3s+1(1)2
     3     -1  7.36421878E+02 1   300   0 1*2 2*7 3*1    2p5 3s1      2p-1(1)1 3s+1(1)0
     4     -1  7.37744083E+02 1   300   2 1*2 2*7 3*1    2p5 3s1      2p-1(1)1 3s+1(1)2
     5     -1  7.54155726E+02 0   301   2 1*2 2*7 3*1    2p5 3p1      2p+3(3)3 3p-1(1)2
     6     -1  7.57795103E+02 0   301   4 1*2 2*7 3*1    2p5 3p1      2p+3(3)3 3p-1(1)4
     7     -1  7.59348028E+02 0   301   6 1*2 2*7 3*1    2p5 3p1      2p+3(3)3 3p+1(3)6
     8     -1  7.60559034E+02 0   301   2 1*2 2*7 3*1    2p5 3p1      2p+3(3)3 3p+1(3)2
     9     -1  7.62368042E+02 0   301   4 1*2 2*7 3*1    2p5 3p1      2p+3(3)3 3p+1(3)4
    10     -1  7.68005929E+02 0   301   0 1*2 2*7 3*1    2p5 3p1      2p+3(3)3 3p+1(3)0
    11     -1  7.69846810E+02 0   301   2 1*2 2*7 3*1    2p5 3p1      2p-1(1)1 3p-1(1)2
    12     -1  7.73062840E+02 0   301   2 1*2 2*7 3*1    2p5 3p1      2p-1(1)1 3p+1(3)2
    13     -1  7.73470206E+02 0   301   4 1*2 2*7 3*1    2p5 3p1      2p-1(1)1 3p+1(3)4
    14     -1  7.90365155E+02 0   301   0 1*2 2*7 3*1    2p5 3p1      2p-1(1)1 3p-1(1)0
    15     -1  8.00169329E+02 1   302   0 1*2 2*7 3*1    2p5 3d1      2p+3(3)3 3d-1(3)0
    16     -1  8.01137358E+02 1   302   2 1*2 2*7 3*1    2p5 3d1      2p+3(3)3 3d-1(3)2
    17     -1  8.02966076E+02 1   302   4 1*2 2*7 3*1    2p5 3d1      2p+3(3)3 3d+1(5)4
    18     -1  8.03096178E+02 1   302   8 1*2 2*7 3*1    2p5 3d1      2p+3(3)3 3d+1(5)8
    19     -1  8.03812355E+02 1   302   6 1*2 2*7 3*1    2p5 3d1      2p+3(3)3 3d-1(3)6
    20     -1  8.05502105E+02 1   302   4 1*2 2*7 3*1    2p5 3d1      2p+3(3)3 3d-1(3)4
```

21	-1	8.06580377E+02	1	302	6	1*2 2*7 3*1	2p5 3d1	2p+3(3)3 3d+1(5)6
22	-1	8.11326891E+02	1	302	2	1*2 2*7 3*1	2p5 3d1	2p+3(3)3 3d+1(5)2
23	-1	8.16455702E+02	1	302	4	1*2 2*7 3*1	2p5 3d1	2p-1(1)1 3d-1(3)4
24	-1	8.17103423E+02	1	302	4	1*2 2*7 3*1	2p5 3d1	2p-1(1)1 3d+1(5)4
25	-1	8.17679088E+02	1	302	6	1*2 2*7 3*1	2p5 3d1	2p-1(1)1 3d+1(5)6
26	-1	8.25272086E+02	1	302	2	1*2 2*7 3*1	2p5 3d1	2p-1(1)1 3d-1(3)2
27	-1	8.60711742E+02	0	300	2	1*2 2*7 3*1	2s1 3s1	2s+1(1)1 3s+1(1)2
28	-1	8.67823477E+02	0	300	0	1*2 2*7 3*1	2s1 3s1	2s+1(1)1 3s+1(1)0
29	-1	8.93685214E+02	1	301	0	1*2 2*7 3*1	2s1 3p1	2s+1(1)1 3p-1(1)0
30	-1	8.94146680E+02	1	301	2	1*2 2*7 3*1	2s1 3p1	2s+1(1)1 3p-1(1)2
31	-1	8.96450212E+02	1	301	4	1*2 2*7 3*1	2s1 3p1	2s+1(1)1 3p+1(3)4
32	-1	8.98437005E+02	1	301	2	1*2 2*7 3*1	2s1 3p1	2s+1(1)1 3p+1(3)2
33	-1	9.38592464E+02	0	302	2	1*2 2*7 3*1	2s1 3d1	2s+1(1)1 3d-1(3)2
34	-1	9.38724254E+02	0	302	4	1*2 2*7 3*1	2s1 3d1	2s+1(1)1 3d-1(3)4
35	-1	9.38975219E+02	0	302	6	1*2 2*7 3*1	2s1 3d1	2s+1(1)1 3d+1(5)6
36	-1	9.43734651E+02	0	302	4	1*2 2*7 3*1	2s1 3d1	2s+1(1)1 3d+1(5)4

```
......
# energy grid
NEGRID = 6
  4.72414560E+01
  5.79761386E+02
  1.39812537E+03
  2.65576771E+03
  4.58848260E+03
  7.55863296E+03
```

```
#lower 2J upper 2J Delta E  nsub
    0  0     1  4  7.2435E+02 1
#The Bethe coefficient and 2 Born coefficients in the Born approximation.
-1.0000E+00  0.0000E+00  0.0000E+00
# if QKMODE = 2, the parameter line is present here.
#user egrid  coll. str.  cross sec.
 4.7241E+01  1.5347E-03  2.3789E-01
 5.7976E+02  9.5137E-04  8.7207E-02
 1.3981E+03  5.1906E-04  2.9211E-02
 2.6558E+03  2.5016E-04  8.8294E-03
 4.5885E+03  1.1322E-04  2.5376E-03
 7.5586E+03  5.1291E-05  7.3523E-04
    0  0     2  2  7.2639E+02 1
 9.1750E-03 -7.0392E-03  7.2655E-03
 4.7241E+01  1.8857E-03  2.9153E-01
 5.7976E+02  3.7280E-03  3.4119E-01
 1.3981E+03  6.3378E-03  3.5633E-01
 2.6558E+03  9.4893E-03  3.3472E-01
 4.5885E+03  1.2996E-02  2.9116E-01
 7.5586E+03  1.6729E-02  2.3974E-01
 ......
```

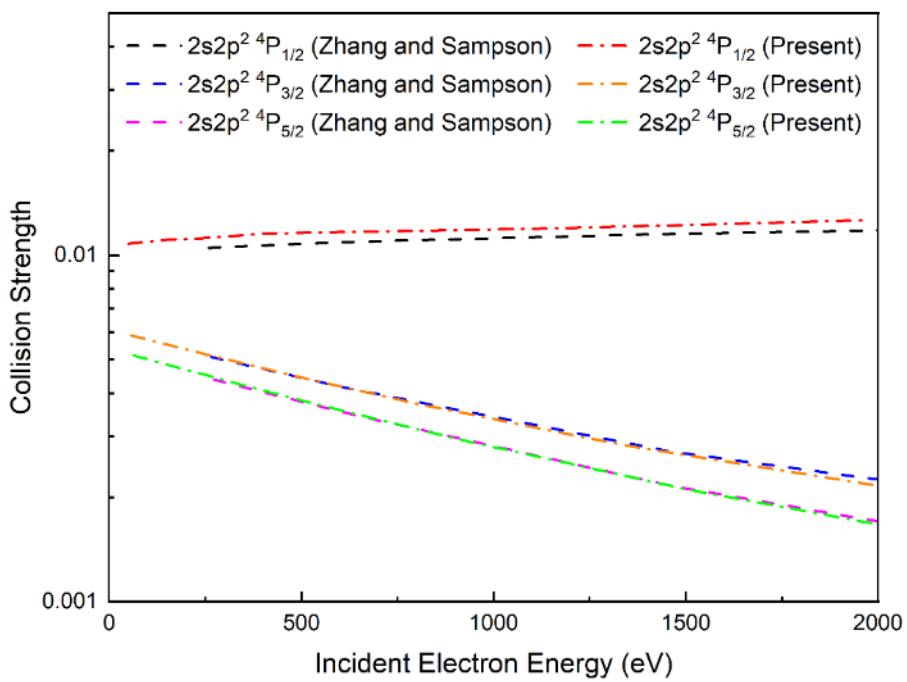
Calculations of Effective collision strengths using JAC

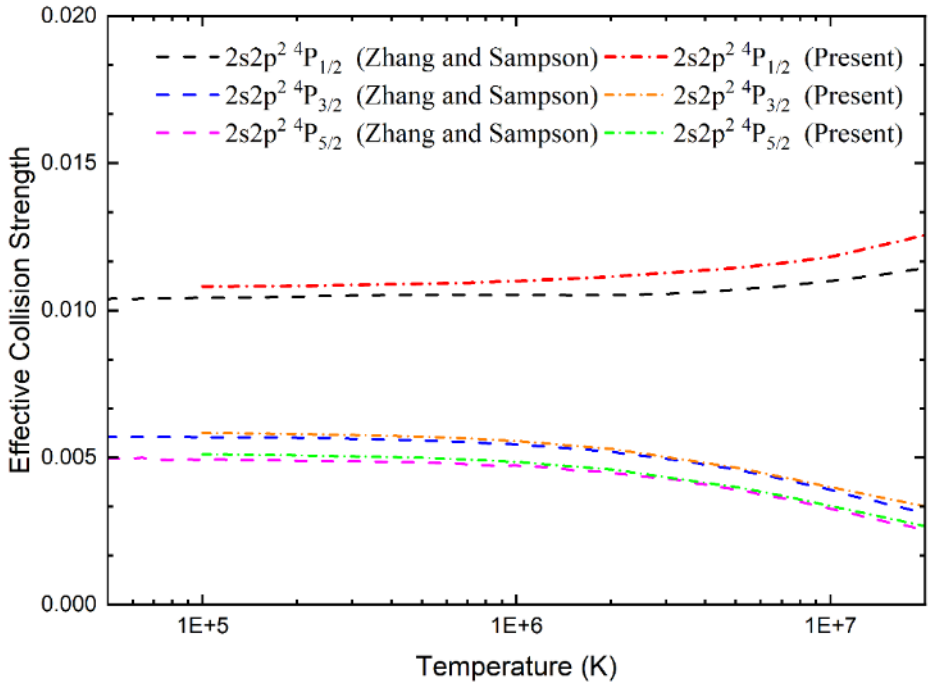
```
# Calculation of effective collision strengths and excitation rate coefficients for Fe XXII
using JAC

# Atomic structure calculations
nucModel = Nuclear.Model(26., "Fermi")
grid = Radial.Grid(Radial.Grid(false), rnt = 4.0e-6, h = 2.5e-2, hp = 2.5e-2, rbox = 30.0)
asfSettings = AsfSettings(AsfSettings(); jjLS=LSjjSettings(true))
wa = Atomic.Computation(Atomic.Computation(),name="Atomic structure calculation - Fe XXII",
                        grid=grid, nuclearModel=nucModel,
                        configs=[Configuration("[He] 2s^2 2p"),Configuration("[He] 2s 2p^2"),
                        Configuration("[He] 2p^3")], asfSettings=asfSettings )
wb = perform(wa; output = true)      ;    multiplet = wb["multiplet:"]     ;

# Effective collision strength and excitation rate coefficient calculations
temps = [1e5, 2e5, 5e5, 7e5, 1e6, 2e6, 5e6, 7e6, 1e7, 2e7]       # temeratures are in Kelvin
settings      = ImpactExcitation.Settings(ImpactExcitation.Settings();
                    lineSelection = LineSelection(true, indexPairs=[(1,3),(1,4),(1,5)]),
                    calcRateCoefficient = true, maxEnergyMultiplier=40., temperatures = temps)

lines, rates = ImpactExcitation.computeLines(multiplet, multiplet, nucModel, grid, settings;
                                                                        output=true);
```

The code is available on GitHub https://github.com/OpenJAC/JAC.jl along with the present extension.

Excitation of Fe XXII using JAC

Collision strengths for the excitations from the ground state of Fe XXII [He] $2s^2 2p\ ^2P_{1/2}$

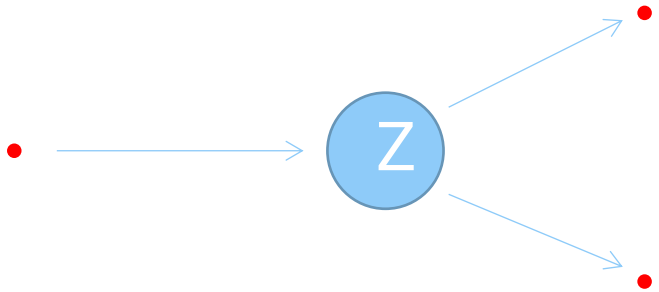


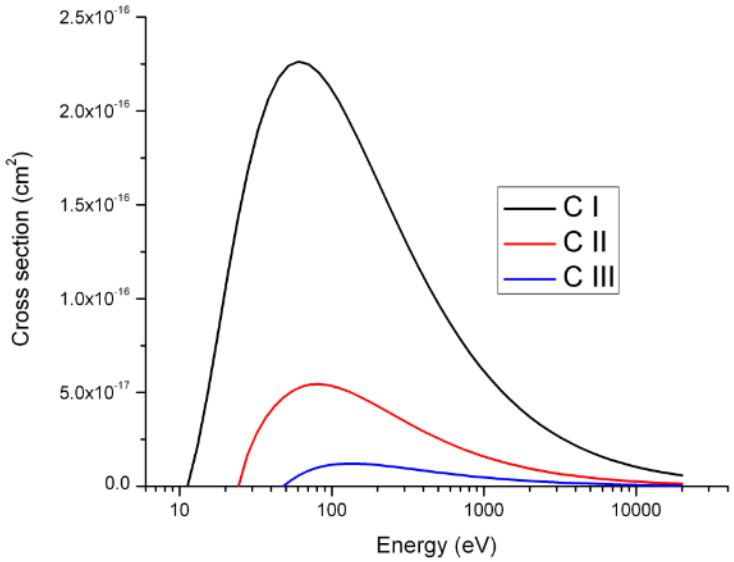


Sahoo, Sharma, Fritzsche, *Eur. Phys. J. Plus (2024) 139:986*

Zhang and Sampson, *Atomic Data and Nuclear Data Tables* **56(1)**, 41–104 (1994)

Electron impact ionization cross sections





$$A + e \rightarrow A^+ + e + e$$

Lotz formula:

$$\sigma_{ion}(n,E) = 2.76\pi \rightleftarrows a_0^2 \frac{Ry^2}{I_n} \frac{\ln(E/I_n)}{E} = 2.76\pi \rightleftarrows a_0^2 \frac{n^4}{Z^4} \frac{\ln X}{X}$$

Same theoretical methods as for excitation: Born, Coulomb-Born, DW, CC, CCC, RMPS…

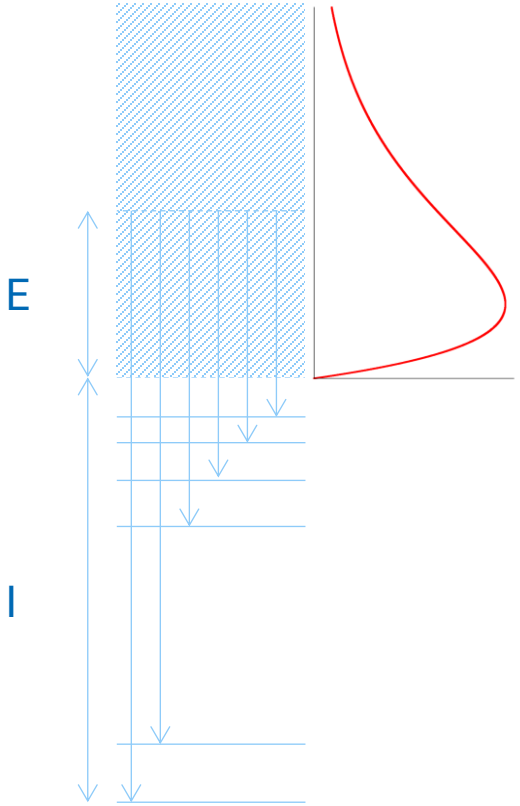
3-Body Recombination

$$A + e \leftrightarrow A^{+} + e + e$$

3-body rate coefficient $\alpha_{Z+1}(T_e)$ from ionization rate coefficient $S_Z(T_e)$:

$$\alpha_{Z+1}(T_e) = \frac{1}{2}\frac{g_z}{g_{z+1}}\left(\frac{2\pi\hbar^2}{m_e T_e}\right)^{3/2} exp\left[\frac{E_z}{T_e}\right] S_Z(T_e)$$

Bound-free:
Radiative Recombination

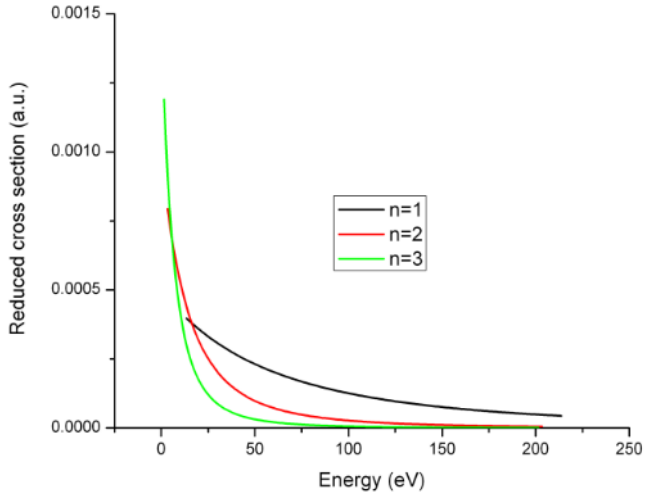


$A^{Z+} + e \rightarrow A^{(Z-1)} + h\nu$ (inverse of photoionization)

$h\nu = E + I$

Semiclassical Kramers cross section: $\sigma_{Kr}(E) = \frac{64\alpha}{3\sqrt{3}} \frac{Z^4}{n^5} \left(\frac{Ry}{E+I} \right)^3 \pi a_0^2$

Quantum-mechanical cross section: $\sigma_{ph}(E) = \sigma_{Kr}(E) \cdot G_n^{bf}(E)$

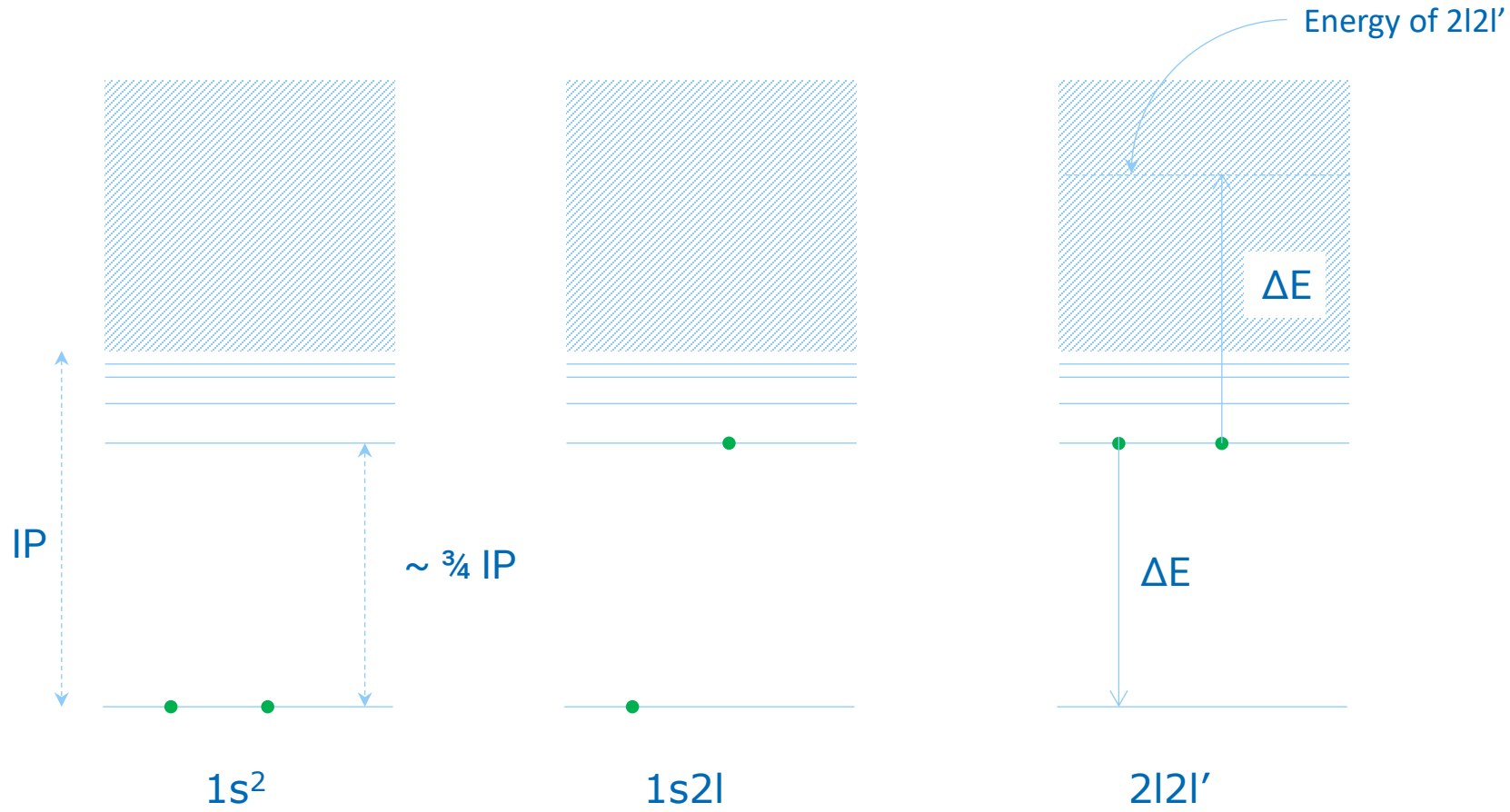


Cross section Z-scaling:

$$\sigma\left(\frac{h\nu}{Z^2}\right) \propto \frac{1}{Z^2}$$

Autoionization

$A^{**} \rightarrow A^{+} + e$



Dielectronic Recombination

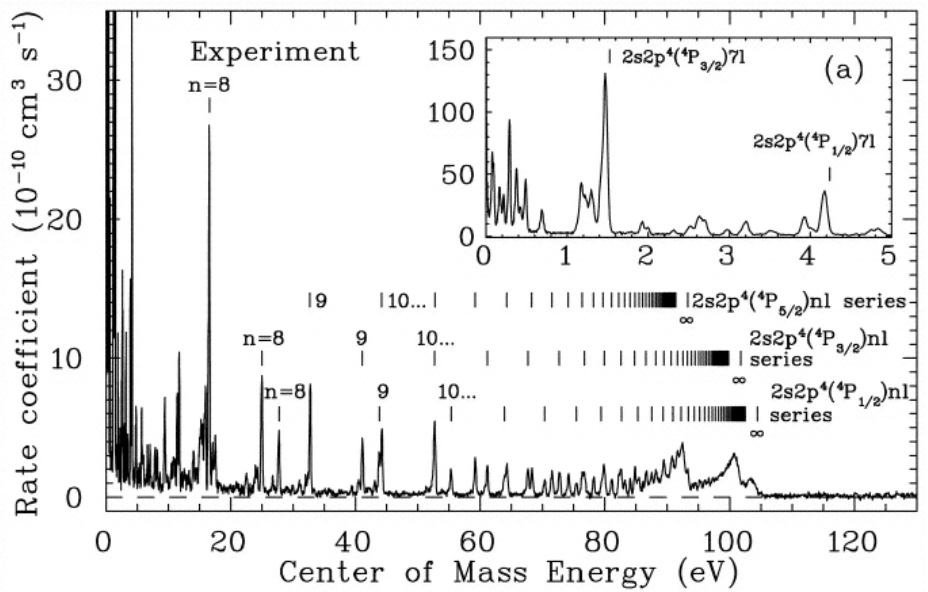
$$A^+ + e \xrightarrow{DC} A^{**} \xrightarrow{AI} A^+ + e$$
$$\downarrow RS$$
$$A^* + h\nu$$

Example: **Δn=0 for Fe XX $2s^22p^3$**

$2s^22p^3\ {}^4S_{3/2} + e \rightarrow 2s2p^4({}^4P_{5/2})nl$

$2s^22p^3\ {}^4S_{3/2} + e \rightarrow 2s2p^4({}^4P_{5/2})nl$

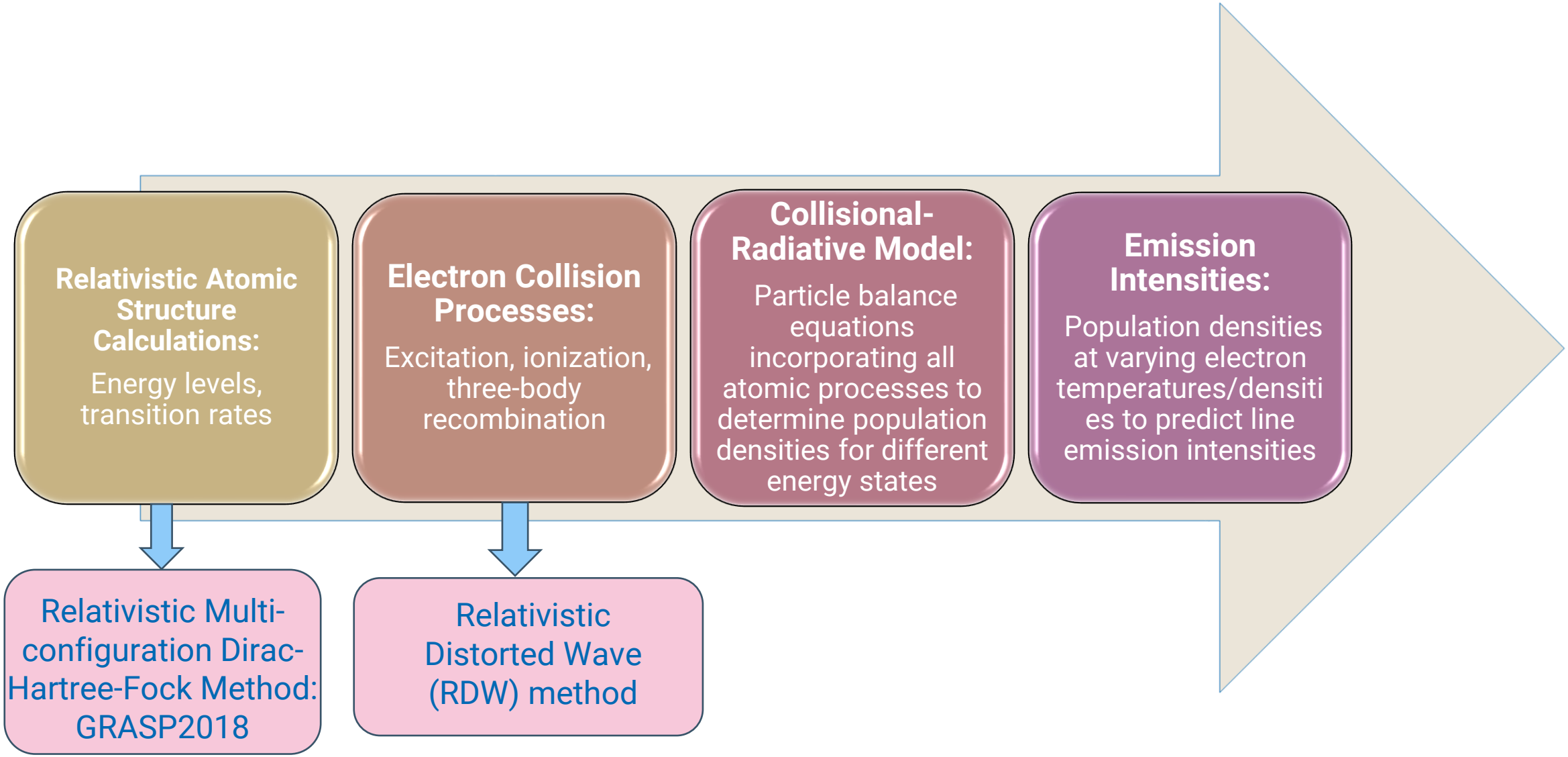
$2s^22p^3\ {}^4S_{3/2} + e \rightarrow 2s2p^4({}^4P_{5/2})nl$



n ≥ 7

Savin et al, 2004

Summary


Relativistic Atomic Structure Calculations:
Energy levels, transition rates
Electron Collision Processes:
Excitation, ionization, three-body recombination
Collisional-Radiative Model:
Particle balance equations incorporating all atomic processes to determine population densities for different energy states
Emission Intensities:
Population densities at varying electron temperatures/densities to predict line emission intensities
Relativistic Multi-configuration Dirac-Hartree-Fock Method: GRASP2018
Relativistic Distorted Wave (RDW) method

Thank You!

fusion-data@iaea.org