Radiative processes

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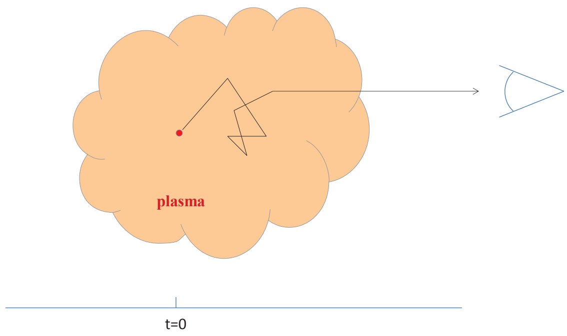
Where are we?..

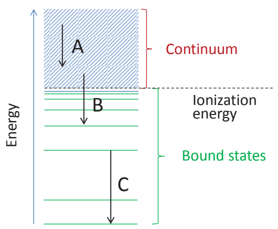


Three major sources of photons

A. Free-free transitions (bremsstrahlung)
   - $A^{z+} + e \rightarrow A^{z+} + e + h\nu$

B. Free-bound transitions (radiative recombination)
   - $A^{z+} + e \rightarrow A^{(z-1)+} + h\nu$

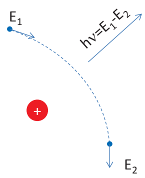
C. Bound-bound transitions
   - $A_j^{z+} \rightarrow A_i^{z+} + h\nu$



Bremsstrahlung (free-free)

- Calculation is straightforward for Maxwellian electrons off bare nuclei of Z:

$$\varepsilon_\lambda^{ff}(\lambda) = \frac{32\sqrt{\pi}c(\alpha a_0)^3 Ry}{3\sqrt{3}} N_Z N_e Z^2 \left(\frac{Ry}{T_e}\right)^{1/2} \frac{1}{\lambda^2} e^{-\frac{hc}{\lambda T_e}} G^{ff}(T_e,\lambda)$$



- Total power loss

$$\varepsilon^{ff} = 4.51\times 10^{-45} Z^2 \left(\frac{T_e}{Ry}\right)^{1/2} N_z N_e \left[\frac{W}{sr\cdot cm^3}\right]$$

- Multicomponent plasma:

$$\varepsilon_\lambda^{ff}(\lambda) = z_{eff}\varepsilon_\lambda^{ff}(\lambda)[H]; \quad z_{eff} = \frac{1}{N_e}\sum_{i,z} z_i^2 N_z^i = \frac{\sum_{i,z} z_i^2 N_z^i}{\sum_{i,z} z_i N_z^i}$$

Dominant at longer wavelengths

Maximum emission at $\lambda_{max} = \frac{620\ nm}{T_e[eV]}$

Bremsstrahlung (cont'd)

$$\varepsilon(\lambda)d\lambda = \varepsilon(\omega)d\omega \qquad \omega = \frac{2\pi c}{\lambda}$$

$$\varepsilon_\omega^{ff}(\omega) = \frac{64c(\alpha a_0)^3 Ry}{3c\sqrt{3\pi}} N_Z N_e Z^2 \left(\frac{Ry}{T_e}\right)^{1/2} e^{-\frac{\hbar\omega}{T_e}} G^{ff}(T_e,\omega)$$

$$\varepsilon_\omega^{ff}(E) \approx A e^{-\frac{E}{T_e}}$$

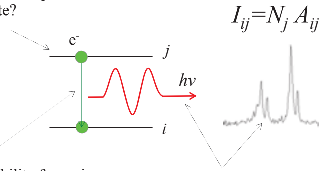
Bound-bound

- Bound-bound transitions between atomic states

A. How many ions in the plasma are in the upper state?

Spectral line intensity

$I_{ij} = N_j A_{ij} h\nu_{ij}$



B. What is the probability for an ion to emit a photon during electron jump?

C. Is the energy of the recorded photon different from that of the emitted one?

These questions are directly related to the environment properties

Spectral Line Intensity

$$I_{ij} = N_j \cdot A_{ij} \cdot E_{ij}$$

- Upper state density (cm^{-3})
- Einstein coefficient or transition probability (s^{-1})
- strongly depends on plasma conditions
- (*almost*) purely atomic parameters
- Energy emitted due to a specific transition from a unit volume per unit time
- Photon energy (erg)

Atomic Processes

Most of related physics is inside this matrix element

$$\left\langle \Psi_f(a',b',c',\ldots) \middle| \hat{O} \middle| \Psi_i(a,b,c,\ldots) \right\rangle$$

final state — interaction operator — initial state

Radiative transitions

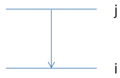
- Classical rate of loss of energy: dE/dt ~ $|\mathbf{a}|^2$, and decay rate ~ $|\mathbf{r}|^2$ for harmonic oscillator
- Quantum treatment: $\langle \Psi_f | \vec{\nabla} \cdot \vec{a}\, e^{i\vec{k}\vec{r}} | \Psi_i \rangle$
  - $e^{ikr} = 1 + ikr + \ldots \approx 1$ (electric dipole or E1 = allowed)
  - Velocity form: $\langle \Psi_f | \nabla | \Psi_i \rangle$
  - Length form: $\langle \Psi_f | r | \Psi_i \rangle$

  must be equal for an exact wavefunction (*good test!*)

- **Spectroscopic charge: Z = ion charge + 1**
  - **e.g. Ar III = Ar^{2+}**
  - **Isoelectronic sequence: different Z_N, same number of electrons. Example: Li-like ions**
    - **Li I, Be II, B III, C IV,…**

S, *f*, and A

- Line strength $S_{ji} = |\langle i \| r \| j \rangle|^2 = S_{ij}$
  - Symmetric w/r to initial-final



- Oscillator strength (*absorption*) $f_{ji} = \frac{1}{3g_i}\frac{\Delta E}{Ry} S$
  - $g_j f_{ij} = g_i f_{ji}$ $\quad (g_j = 2J_j + 1)$; dimensionless
  - Typical values for strong lines: **~ 0.1-1**
- Transition probability (or Einstein coefficient)

$$A_{ij} = 4.3 \cdot 10^7 \frac{g_i}{g_j} (\Delta E[eV])^2 f_{ji}$$

$$A_{ij} = \frac{2h\nu^3}{c^2} B_{ij},\; g_j B_{ij} = g_i B_{ji}$$

  - Typical values for neutrals: ~ 10^8 s^{-1}

$\tau = 1/A$

Selection rules and Z-scaling

Fundamental law: parity and J do not change

Before: P_j $\quad \vec{J}_j$

After: $P_i \cdot P_{ph}$ $\quad \vec{J}_i + \vec{J}_{ph}$

$P_{ph} = -1$
$J_{ph}(E1) = 1$

Exact selection rules:
$P_j = -P_i$
$|\Delta J| \le 1$, $0 \not\to 0$ $(J_j + J_i \ge 1)$

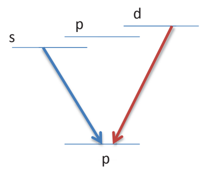
Approximate selection rules (for LS coupling):
$\Delta S = 0$, $|\Delta L| \le 1$, $0 \not\to 0$

Intercombination transitions: $\Delta S \neq 0$
$2s^2\ {}^1S_0 - 2s2p\ {}^3P_1$

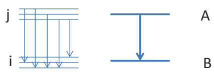
- **Δn ≠ 0**
  - $r \propto Z^{-1} \Rightarrow S \propto Z^{-2}$
  - $\Delta E \propto Z^2 \Rightarrow f \propto Z^0$
  - $A \propto Z^4$
- **Δn = 0**
  - $r \propto Z^{-1} \Rightarrow S \propto Z^{-2}$
  - $\Delta E \propto Z \Rightarrow f \propto Z^{-1}$
  - $A \propto Z$

Some useful info

- "Left" is stronger than "right"
  - $f(\Delta l = -1) > f(\Delta l = +1)$
  - He I
    - $f(1s2p\ {}^1P_1 - 1s3s\ {}^1S_0) = 0.049$
    - $f(1s2p\ {}^1P_1 - 1s3d\ {}^1D_2) = 0.71$



- Level grouping
  - Average over initial states
  - Sum over final states
  - *Example: from levels to terms*
  - Any physical parameter



$$\alpha_{BA} = \sum_i \frac{\sum_j g_j \alpha_{ij}}{\sum_j g_j}$$

Principal quantum number n

- *n*-dependence for *f*

$$f(n_1 \to n_2) \approx \frac{32}{3\pi\sqrt{3}} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)^{-3} \frac{1}{n_1^5} \frac{1}{n_2^3}$$

$$f(\Delta n = 1) \approx \frac{4}{3\pi\sqrt{3}} n \approx 0.245 n$$

$$f(n_2 >> n_1) \propto \frac{1}{n_2^3}$$

- *n*-dependence for A

$$A(n_2 >> n_1) \propto \frac{1}{n_2^3}$$

- Total radiative rate from a specific *n*

$$A_Z(n) \approx 1.6 \times 10^{10} \frac{Z^4}{n^{9/2}}$$

Forbidden transitions (high multipoles)

- QED: En, Mn (n=1, 2,…)
- E1/M1 dipole, E2/M2 quadrupole, E3/M3 octupole,…
- *Selection rules*
  - $P_j \cdot P_i$
    - **+1** for M1, E2, M3,…
    - **-1** for E1, M2, E3,…
  - $J_{ph}(En/Mn) = n$
- M3 and E3 were measured!
- Magnetic dipole (M1)
  - Stronger within the same configuration/term
  - **A ∝ Z^6 or stronger**
  - Same parity, $|\Delta J| \le 1$, $J_j + J_i \ge 1$
- Electric quadrupole (E2)
  - Stronger between configurations/terms
  - **A ∝ Z^6 or stronger**
  - Same parity, $|\Delta J| \le 2$, $J_j + J_i \ge 2$

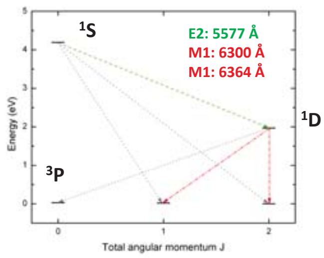
Generally weak…

Aurora borealis

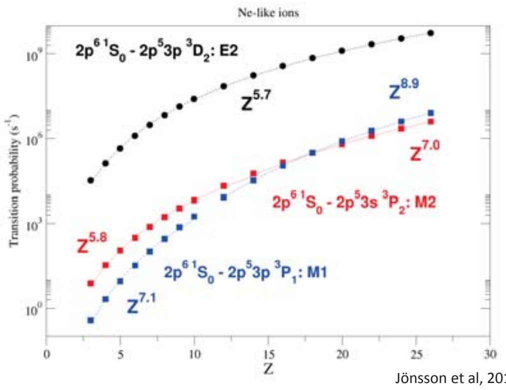
Forbidden transitions: auroras

Wavelength	Transition	A(s^{-1})
2958	$^1S_0$-$^3P_2$	E2: 2.42(-4)
2972	$^1S_0$-$^3P_1$	M1: 7.54(-2)
5577	**$^1S_0$-$^1D_2$**	**E2: 1.26(+0)**
6300	**$^1D_2$-$^3P_2$**	**M1: 5.63(-3)**
6300	$^1D_2$-$^3P_2$	E2: 2.11(-5)
6364	**$^1D_2$-$^3P_1$**	**M1: 1.82(-3)**
6364	$^1D_2$-$^3P_1$	E2: 3.39(-6)
6392	$^1D_2$-$^3P_0$	E2: 8.60(-7)

O I $2p^4$

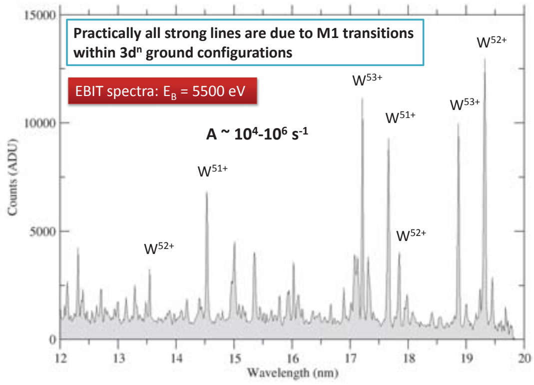


Scaling in Ne-like ions

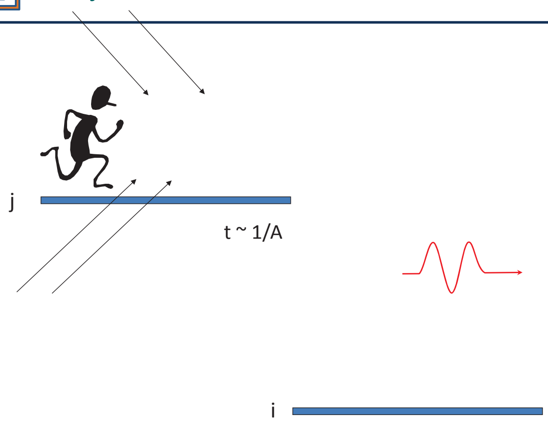


Jönsson et al, 2011

Forbidden transitions: highly-charged W



Why are the forbidden lines sensitive to density?



Atomic Structure Methods and Codes

- Coulomb approximation (Bates-Darmgaard)
- Single-configuration Hartree-Fock (self-consistent field)
  - Cowan's code, online interfaces available
- Model potential (including relativistic)
  - **HULLAC**, **FAC**, AUTOSTRUCTURE
- Multiconfiguration HF (`http://nlte.nist.gov/MCHF`)
- Multiconfiguration Dirac-Fock (MCDF)
  - GRASP2K (`http://nlte.nist.gov/MCHF`)
  - Desclaux's code
- Various perturbation theory methods
- B-splines

http://plasma-gate.weizmann.ac.il/directories/free-software/

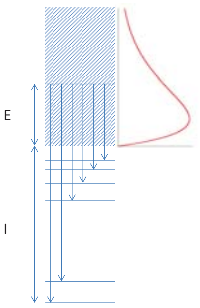
Atomic Structure & Spectra Databases

- Extensive list
  - http://plasma-gate.weizmann.ac.il/directories/databases/
- Evaluated and recommended data
  - NIST Atomic Spectra Database http://physics.nist.gov/asd
    - Level energies, ionization potentials, spectral lines, transition probabilities
- Other data collections
  - VALD (Sweden)
  - SPECTR-W3 (Russia)
  - CAMDB (China)
  - CHIANTI (USA/UK/…)
  - Kurucz databases (USA)
  - GENIE (IAEA)
  - …

Short introduction to ASD

- Contents
- Lines: Fe XXV; uncertainty; intensity; bibliography; Grotrian

Radiative Recombination

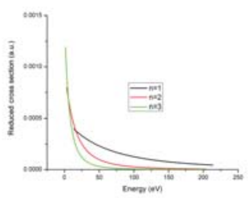


$A^{Z+} + e \rightarrow A^{(Z-1)} + h\nu$ (inverse of photoionization)

$h\nu = E + I$

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

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

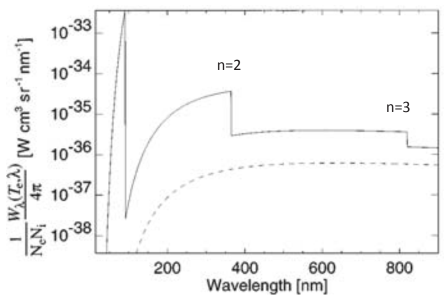


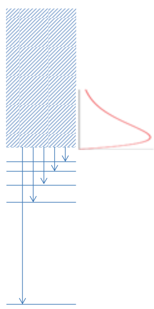
Cross section Z-scaling:

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

FF+BF at Alcator C-mod: 1 eV, H

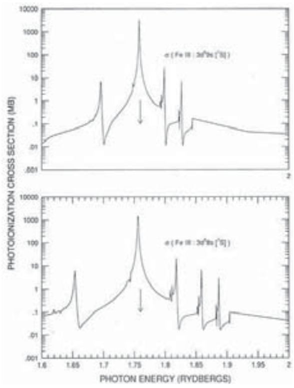
Edge:





Lumma et al (1997)

Resonances in photoionization



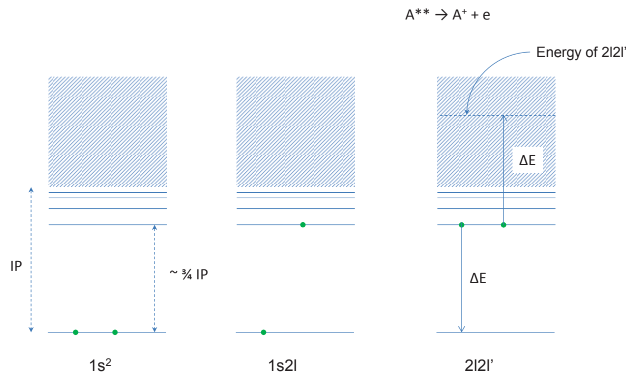
Fe III

$3d^5(^6S)ns\ ^7S + h\nu \to 3d^5\ ^6S$

$3d^5(^6S)ns\ ^7S + h\nu \to 3d^44p(^4P^o)ns\ ^7P^o \to 3d^5\ ^6S$

A. Pradhan

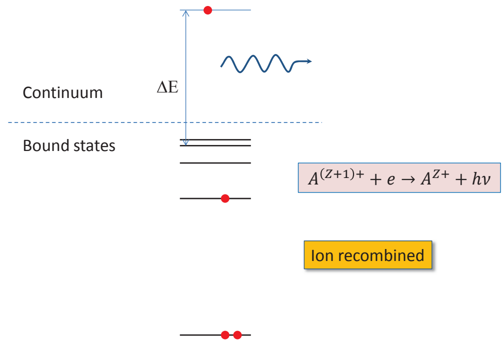
Autoionization



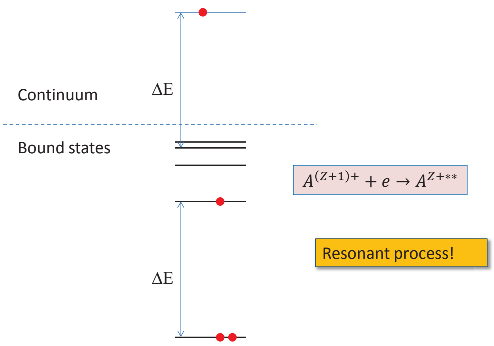
Selection rules

- Examples of AI states: $1s2s^2$, $1s^22pnl$ (high n)
- Same old rule: **before** = **after**
- $A^{**} \to A^* + \varepsilon l$
  - ***Exact***: $P_j = P_i$; $\Delta J = 0$
  - *Approximate* (LS coupling): $\Delta S = 0$, $\Delta L = 0$
- $2p^2\ ^3P \to 1s + \varepsilon p$: *parity/L violation*!
  - BUT: $\Psi(2p^2\ ^3P_2) = \alpha\Psi(2p^2\ ^3P_2) + \beta\Psi(2p^2\ ^1D_2) + \ldots$
  - and $\Psi(2p^2\ ^3P_0) = \alpha'\Psi(2p^2\ ^3P_0) + \beta'\Psi(2p^2\ ^1S_0) + \ldots$
  - YET: $A_a(2p^2\ ^3P_1) \approx 0$

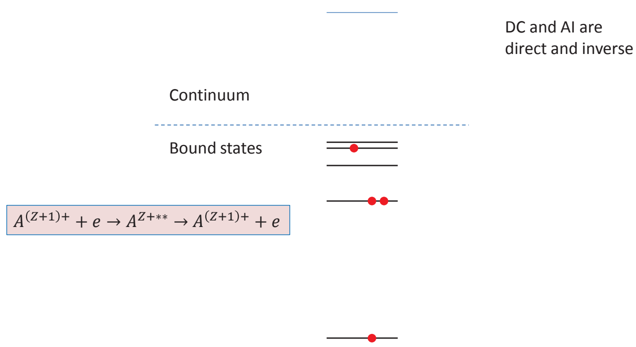
Radiative recombination



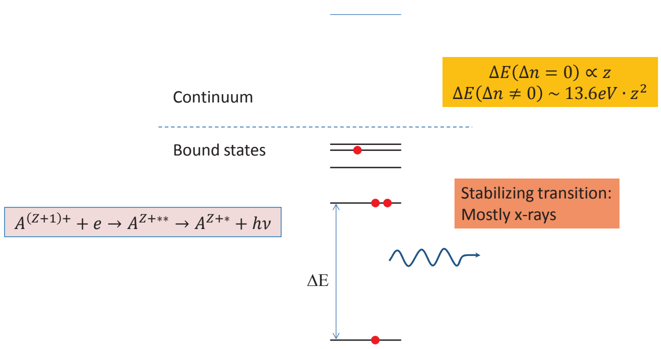
DR step 1: dielectronic capture



Dielectronic capture + autoionization = **no recombination**



DR step 2: radiative stabilization

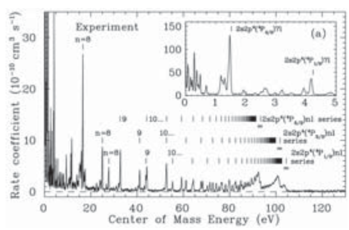


Dielectronic Recombination

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

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

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



$n \geq 7$

Savin et al, 2004

Dielectronic Recombination

$A^{+}+e \xrightarrow{DC} A^{**} \xrightarrow{AI} A^{+}+e$

$\downarrow$ RS

$A^{*}+h\nu$

Examples:

$1s^2 + e \rightarrow 1s2pnl \rightarrow 1s^2nl + h\nu$

$1s^22s^2 + e \rightarrow 1s^22s2pnl \rightarrow 1s^22s^2nl + h\nu$

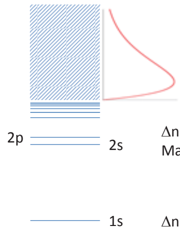
$1s^22s^2 + e \rightarrow 1s2s^22pnl \rightarrow 1s^22s^2nl + h\nu$

$1s^2 + e \rightarrow 1s2pnl \rightarrow 1s^2nl + h\nu$

$1s^22s + e \rightarrow 1s^22pnl \rightarrow 1s^22snl + h\nu$

$1s^22s + e \rightarrow 1s^23pnl \rightarrow 1s^22snl + h\nu$

$1s^22s + e \rightarrow 1s2s2pnl \rightarrow 1s^22snl + h\nu$

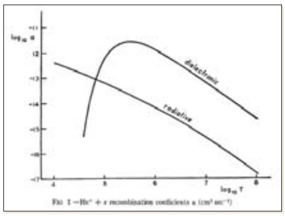


Δn=0: high n important, Major difficulty: n→∞

Δn>0: high n not as important

Examples of dielectronic recombination & resonances

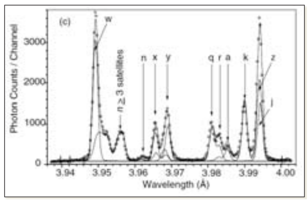
He⁺ + e



A. Burgess, ApJ **139**, 776 (1964)

This work solved the ionization balance problem for solar corona

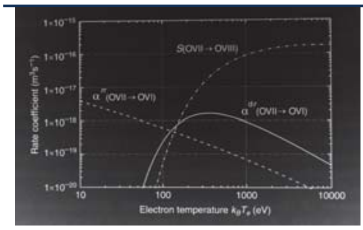
Dielectronic satellites are important for plasma diagnostics (e.g., He- and Li-like ions)



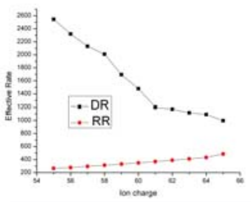
Ar at NSTX, Bitter et al (2004)

BUT: DR for high-Z multi-electron ions is barely known!

Is DR important?..



RR and DR for O VII (Kunze, 2009)



W ions: T_e = 9000 eV, $N_e = 10^{14}$ cm^{-3} (NLTE-7 Workshop, unpublished)

Answer: YES

Burgess (1964) was the first to show importance of DR for solar corona ionization balance

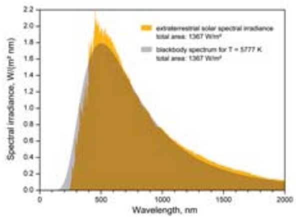
There exist a number of recommended formulas for rate coefficients of variable quality; **Z < 30** (Burgess-Merts-Magee-Cowan, Badnell et al, Mazzotta et al, Hahn, Gu,…)

$$\alpha_{DR} = \frac{1}{T_e^{3/2}} \sum_i C_i \exp\left(-\frac{E_i}{T_e}\right)$$

Planck and Maxwell

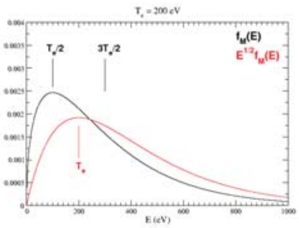
- Planck distribution

$$B(E) = \frac{2E^3}{h^2c^2}\frac{1}{e^{E/T}-1}$$

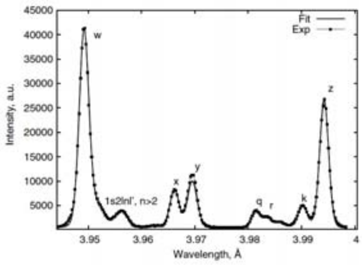


- Maxwell distribution

$$f_M(E)dE = \frac{2}{\pi^{1/2}T_e^{3/2}}E^{1/2}\exp\left(-\frac{E}{T_e}\right)dE$$



He-like lines and satellites

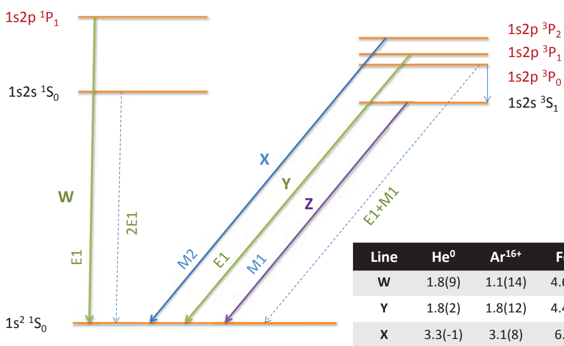


O.Marchuk et al, J Phys B 40, 4403 (2007)

Energy levels in He-like Ar

- Ground state: $1s^2\ ^1S_0$
- Two subsystems of terms
  - Singlets **1s*nl* ¹L**, J=*l* (example $1s3d\ ^1D_2$)
  - Triplets **1s*nl* ³L**, J=*l*-1,*l*,*l*+1 (example $1s2p\ ^3P_{0,1,2}$)
- Radiative transitions within each subsystem are strong, between systems depend on Z

He-like Ar Levels and Lines

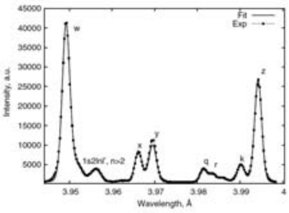


Line	He^0	Ar^{16+}	Fe^{25+}	Kr^{34+}
W	1.8(9)	1.1(14)	4.6(14)	1.5(15)
Y	1.8(2)	1.8(12)	4.4(13)	3.9(14)
X	3.3(-1)	3.1(8)	6.5(9)	9.3(10)
Z	1.3(-4)	4.8(6)	2.1(8)	5.8(9)

Z-scaling of A's

- W[E1]: $A(1s^2\ ^1S_0 - 1s2p\ ^1P_1) \propto \mathbf{Z^4}$
- Y[E1]: $A(1s^2\ ^1S_0 - 1s2p\ ^3P_1)$
  - $\propto \mathbf{Z^{10}}$ for low Z
  - $\propto \mathbf{Z^{8}}$ for large Z
  - $\propto \mathbf{Z^{4}}$ for very large Z
- X[M2]: $A(1s^2\ ^1S_0 - 1s2p\ ^3P_2) \propto \mathbf{Z^8}$
- Z[M1]: $A(1s^2\ ^1S_0 - 1s2s\ ^3S_1) \propto \mathbf{Z^{10}}$

1*s*2*lnl* satellites



- 1l2l2l'
  - 1s2s^2: $^2S_{1/2}$
  - 1s2s2p:
    - 1s2s2p(^{1}P) $^2P_{1/2,3/2}$
    - 1s2s2p(^{3}P) $^2P_{1/2,3/2}$; $^4P_{1/2,3/2,5/2}$
  - 1s2p^2
    - 1s2p^2(^{1}D) $^2D_{3/2,5/2}$
    - 1s2p^2(^{3}P) $^2P_{1/2,3/2}$; $^4P_{1/2,3/2,5/2}$
    - 1s2p^2(^{1}S) $^2S_{1/2}$
- 1s2lnl'
  - Closer and closer to W
  - Only 1s2l3l can be reliably resolved
  - Contribute to W line profile