# Atomic Line Intensities and Collisional-Radiative Modeling

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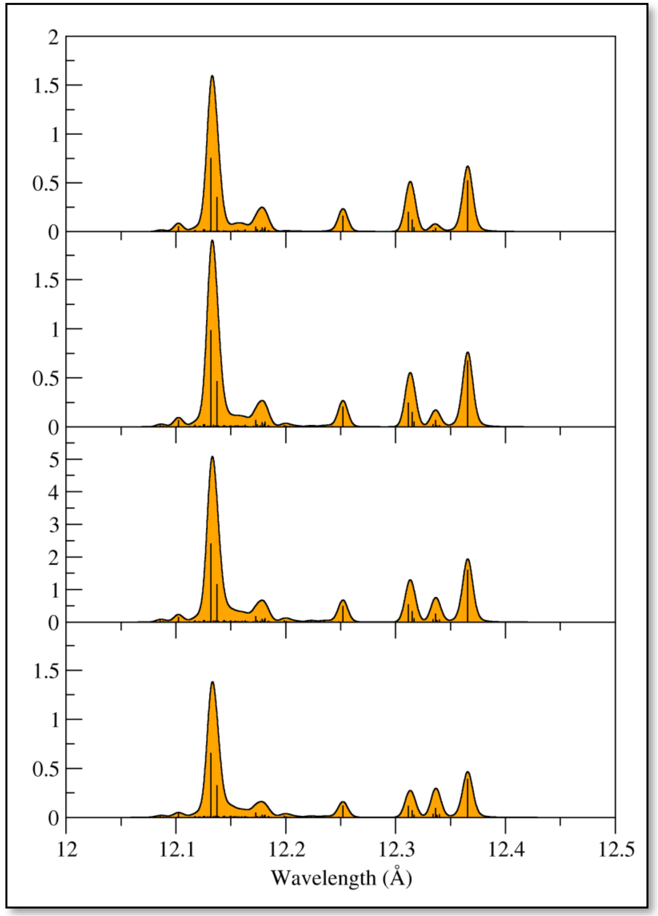


Joint ICTP-IAEA School on Atomic and Molecular Processes in Plasmas
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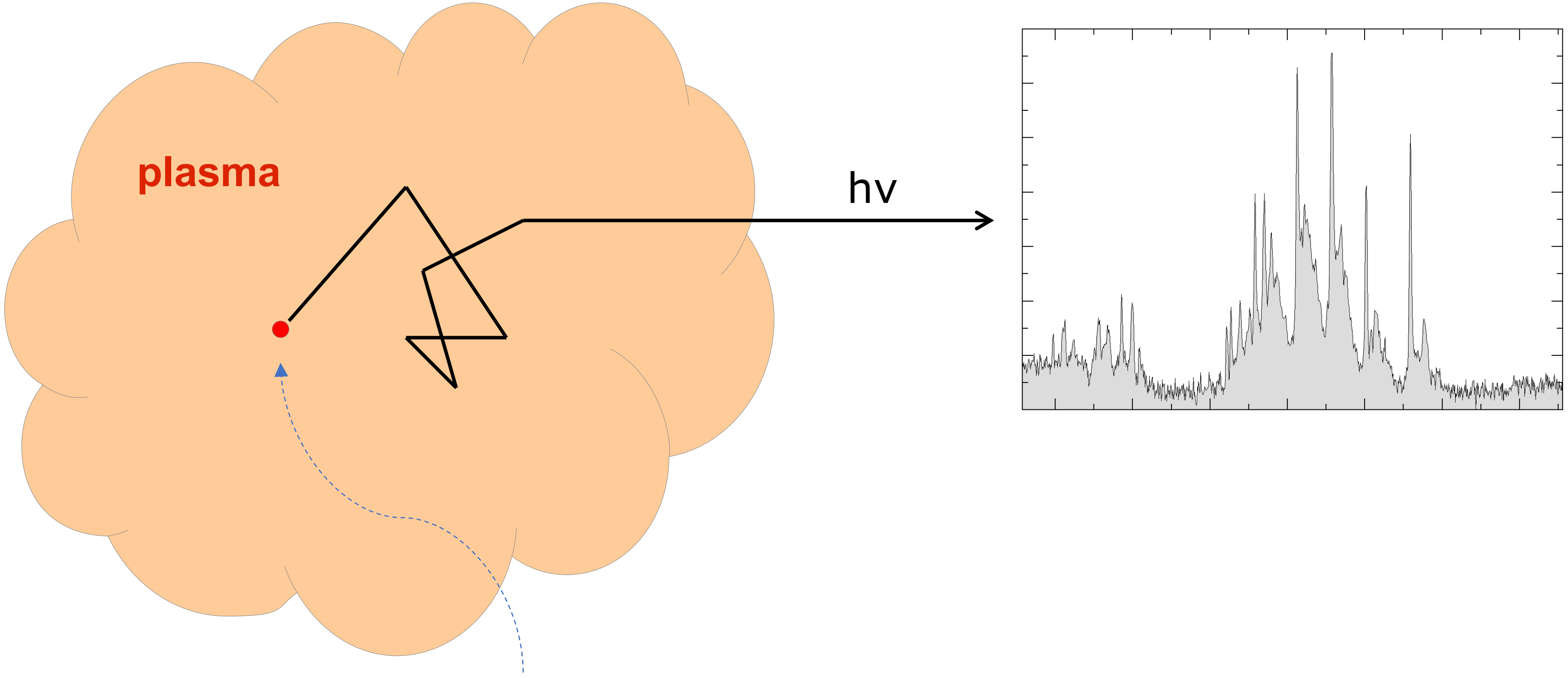
# Back to the photon's life




What happens here?

# Example: Spectral Line Intensity

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

Upper state density ($cm^{-3}$)

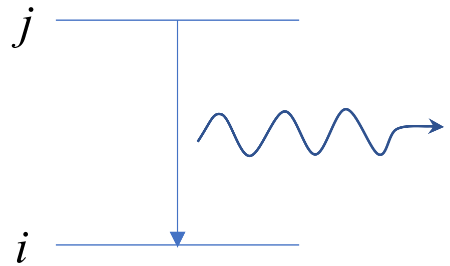
strongly depends
on plasma conditions

Einstein coefficient or
transition probability ($s^{-1}$)

(*almost*) purely
atomic parameters

Energy emitted due to a specific
transition from a unit volume
per unit time

Photon energy (eV)



# Rates

velocity (or energy) distribution function [s/cm]

relative velocity [cm/s]

**Collisional**:

$$R_{ij} = N_p \cdot \int \mathrm{v} \cdot \sigma_{ij}(\mathrm{v}) \cdot f_p(\mathrm{v})\, d^3\mathrm{v}$$

[$s^{-1}$]

projectile density [$cm^{-3}$]

cross section [$cm^2$]

---

**Radiative and Autoionization**:

A [$s^{-1}$]

Lifetime = 1/A [s]

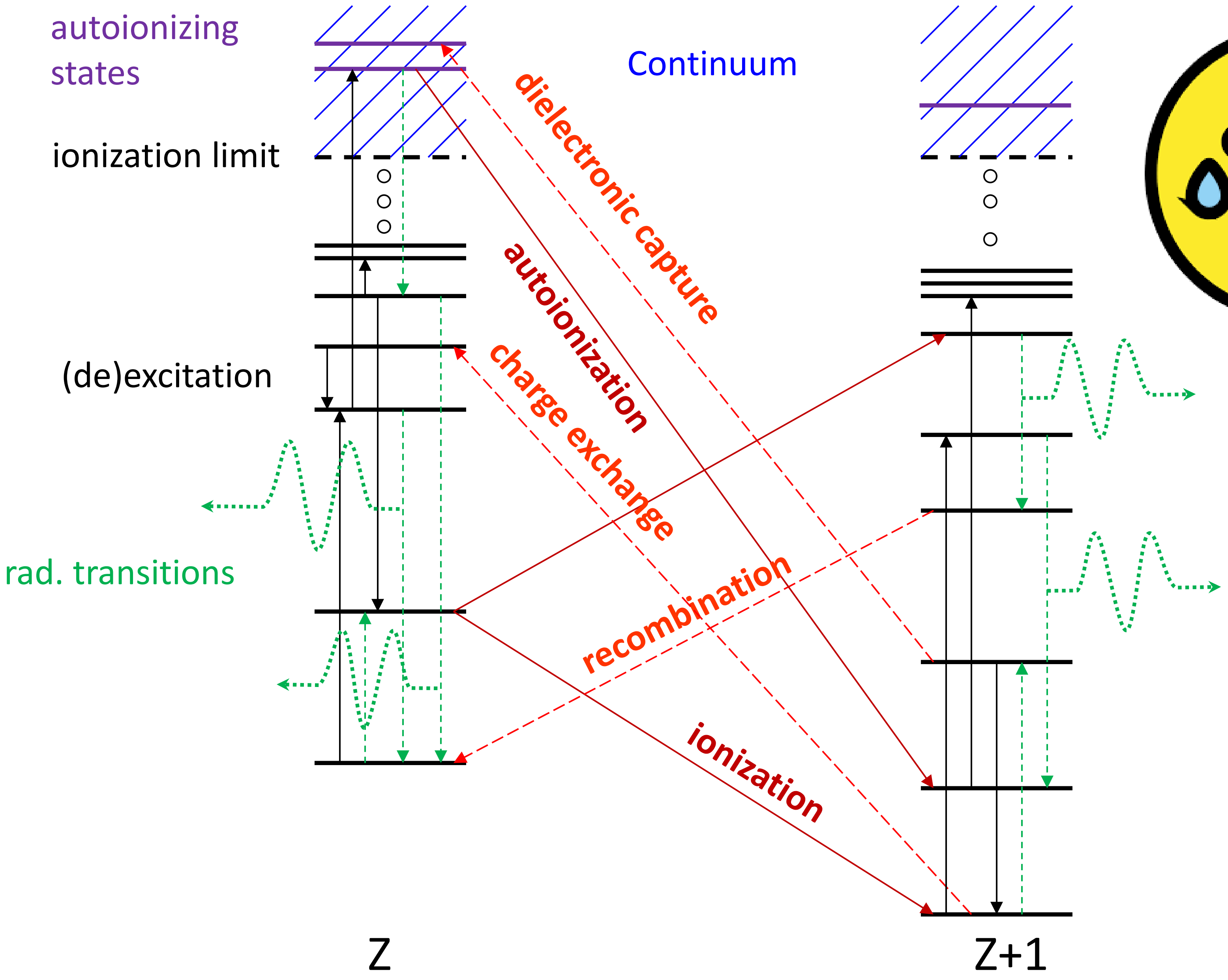
# Z-scalings of atomic parameters

- Radiative ($A \sim f \cdot \Delta E^2$)
  - **$\Delta n = 0$**
    - **$\Delta E \sim Z$**
    - **$f \sim Z^{-1}$**
    - **$A \sim Z$**
  - **$\Delta n \neq 0$**
    - **$\Delta E \sim Z^2$**
    - **$f \sim Z^0$**
    - **$A \sim Z^4$**
  - ***n*-dependence**
    - **$f \sim n^{-3}$**
    - **$A \sim n^{-3}$**

E1 only! Forbidden: $Z^6$-$Z^{12}$

- Collisional ($\sigma \sim f/\Delta E^2$)
  - **$\Delta n = 0$**
    - **$\sigma \sim Z^{-3}$**
    - **$\langle \sigma \cdot v \rangle \sim Z^{-2}$**
  - **$\Delta n \neq 0$**
    - **$\sigma \sim Z^{-4}$**
    - **$\langle \sigma \cdot v \rangle \sim Z^{-3}$**
  - ***n*-dependence**
    - **$\sigma \sim n^{-3}$**
    - **$\sigma(\Delta n = 1) \sim n^4$**

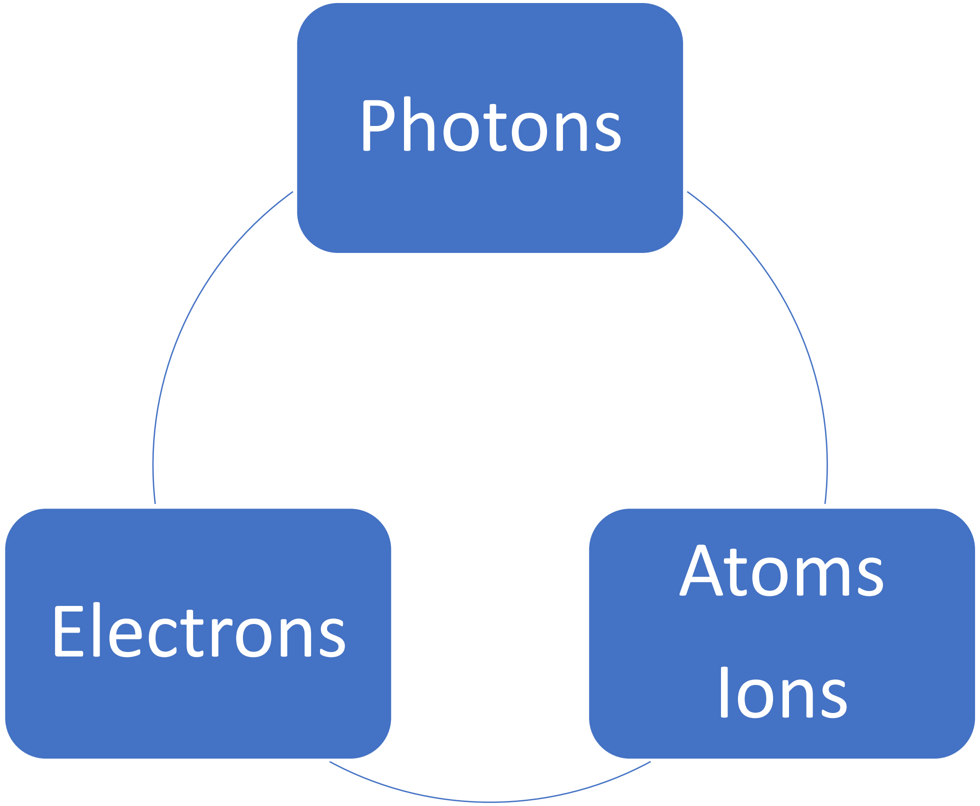
# There are so many processes…



# Thermodynamic equilibrium

Principle of detailed balance

- ***each direct process is balanced by the inverse***
  - excitation ↔ deexcitation
  - ionization ↔ 3-body recombination
  - photoionization ↔ photorecombination
  - autoionization ↔ dielectronic capture
  - radiative decay (spontaneous+stimulated) ↔ photoexcitation

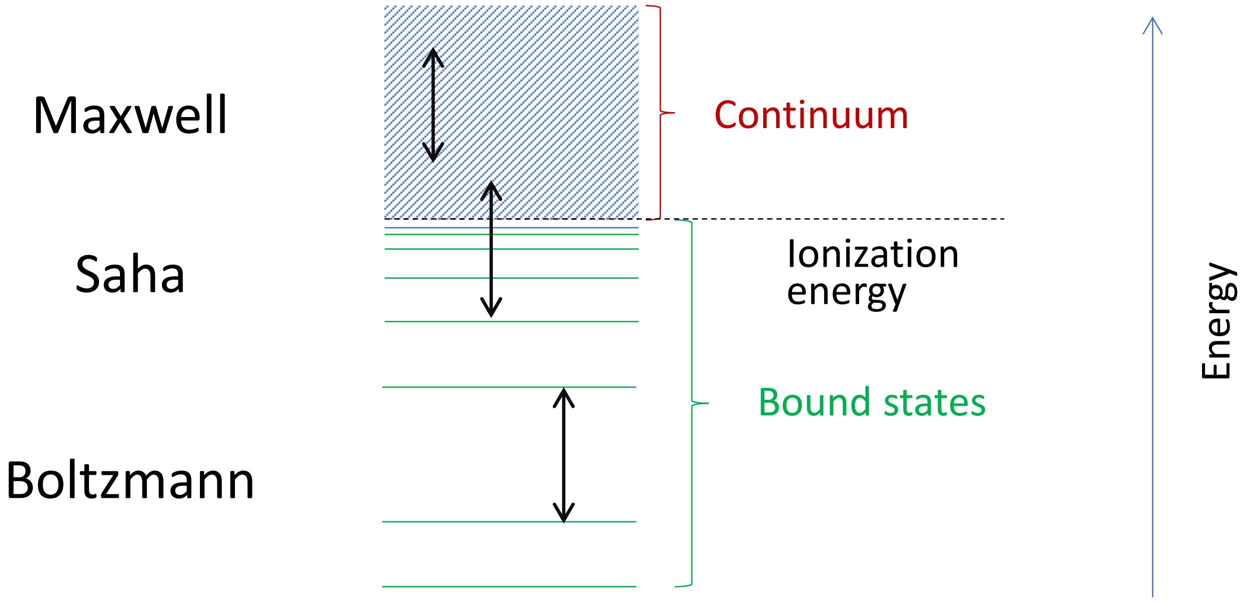


# TE: distributions

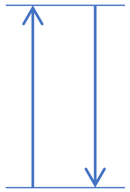
- Four "systems": **photons**, **electrons**, **atoms** and **ions**
- Same temperature $T_r = T_e = T_i$
- We know the equilibrium distributions for each of them
  - Photons: Planck
  - Electrons: Maxwell
  - Populations within atoms/ions: Boltzmann
  - Populations between atoms/ions: Saha

Excellent review: J.A.M. van der Mullen, *Phys. Rep.* **191**, 109 (1990)

# Thermodynamic equilibrium: energy scheme



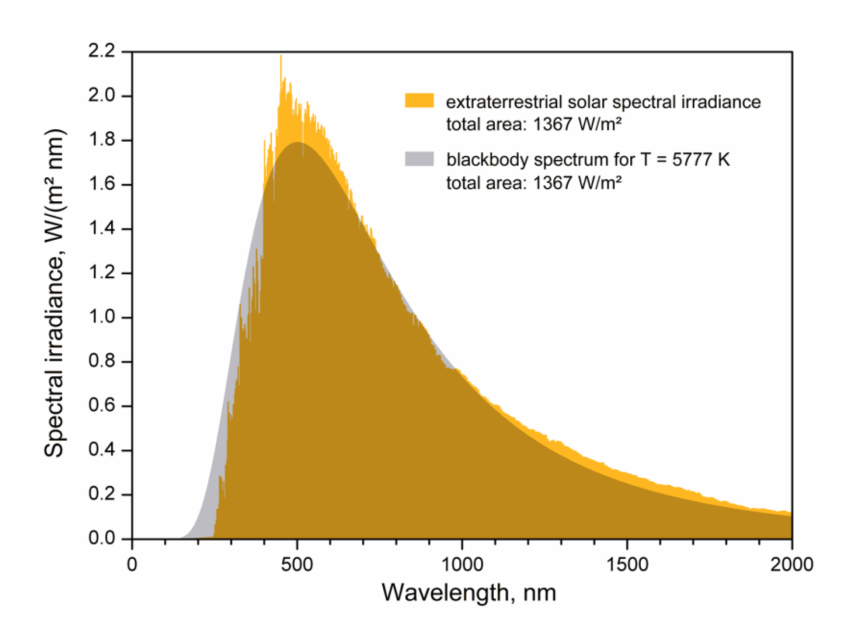

Everything is "Boltzmann:" $\frac{N_1}{N_2} = \frac{g_1}{g_2} \exp\left(-\frac{E_1 - E_2}{T_e}\right)$



# Planck and Maxwell

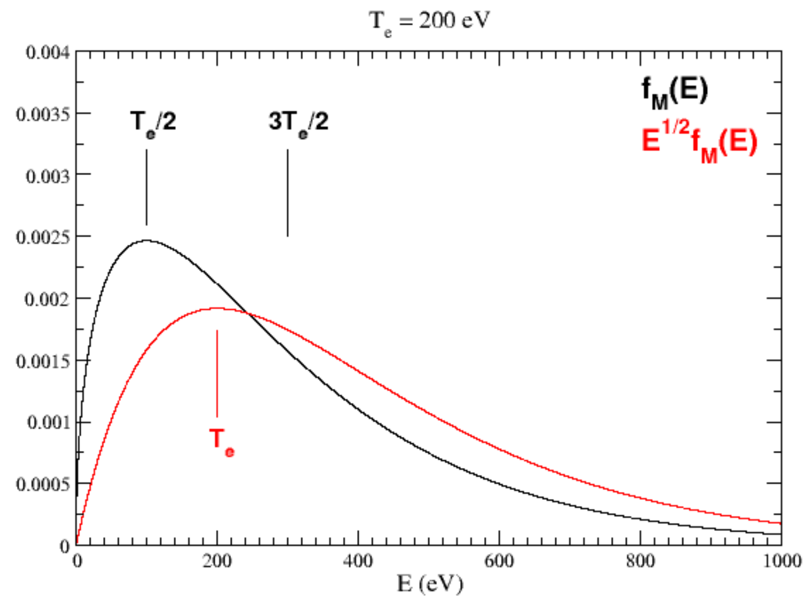
- Planck distribution

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



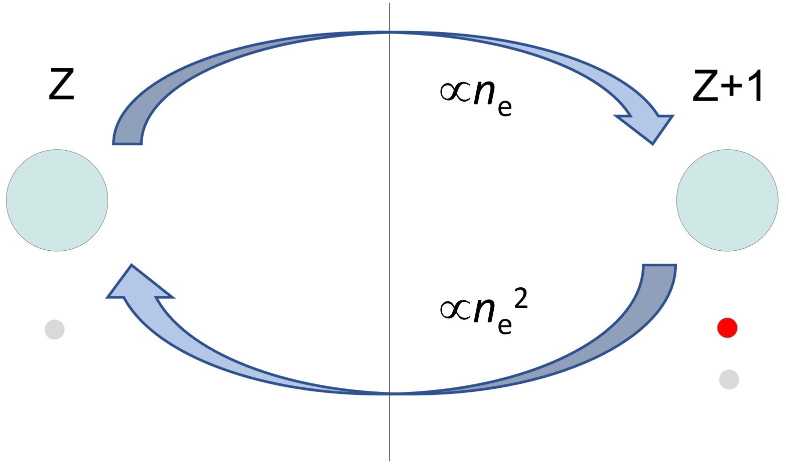

- Maxwell distribution

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



# Saha Distribution

$A_Z$ (+ e) $\leftrightarrow$ $A_{Z+1}$ + e (+ e)




ionization ⟷ 3-body recombination

autoionization ⟷ dielectronic capture

$$\frac{N^{Z+1}}{N^Z} = \frac{g_{Z+1}}{g_Z} 2 \left(\frac{2\pi m T_e}{h^2}\right)^{3/2} \frac{1}{n_e} e^{-\frac{I_Z}{T_e}}$$

$$g_Z = \sum_i g_{Z,i} e^{-\frac{E_i - E_0}{T_e}}$$

Which ion is the most abundant?

$$\frac{N^{Z+1}}{N^Z} = 1 \qquad \frac{I_Z}{T_e} >> 1 \ (\sim 10)$$

# Local Thermodynamic Equilibrium

- **(Almost) never complete TE**: photons decouple easily…therefore, let's forget about the photons!
- LTE = Saha + Boltzmann + **Maxwell**
- McWhirter's's criterion for Boltzmann: *collisional rates > 10*radiative rates*

$$n_e[cm^{-3}] > 1.7 \times 10^{14} (\Delta E_{01}[eV])^3 (T_e[eV])^{1/2} \propto Z^7$$

H I (2 eV): $2 \times 10^{17}$ cm$^{-3}$
C V (80 eV): $2 \times 10^{22}$ cm$^{-3}$

- Saha criterion **for low $T_e$**

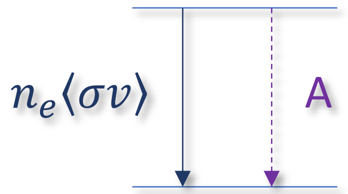
$$n_e[cm^{-3}] > 1 \times 10^{14} (I_z[eV])^{5/2} (T_e[eV])^{1/2} \propto Z^6$$

H I (2 eV): $10^{17}$ cm$^{-3}$
C V (80 eV): $3 \times 10^{21}$ cm$^{-3}$

# McWhirter's criterion

$$n_e[cm^{-3}] > 1.6 \times 10^{12} (\Delta E_{01}[eV])^3 (T_e[K])^{1/2}$$

$$n_e[cm^{-3}] > 1.7 \times 10^{14} (\Delta E_{01}[eV])^3 (T_e[eV])^{1/2}$$




$$n_e\langle\sigma v\rangle > 10A$$

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

($\bar{g} = 0.2$) for ions

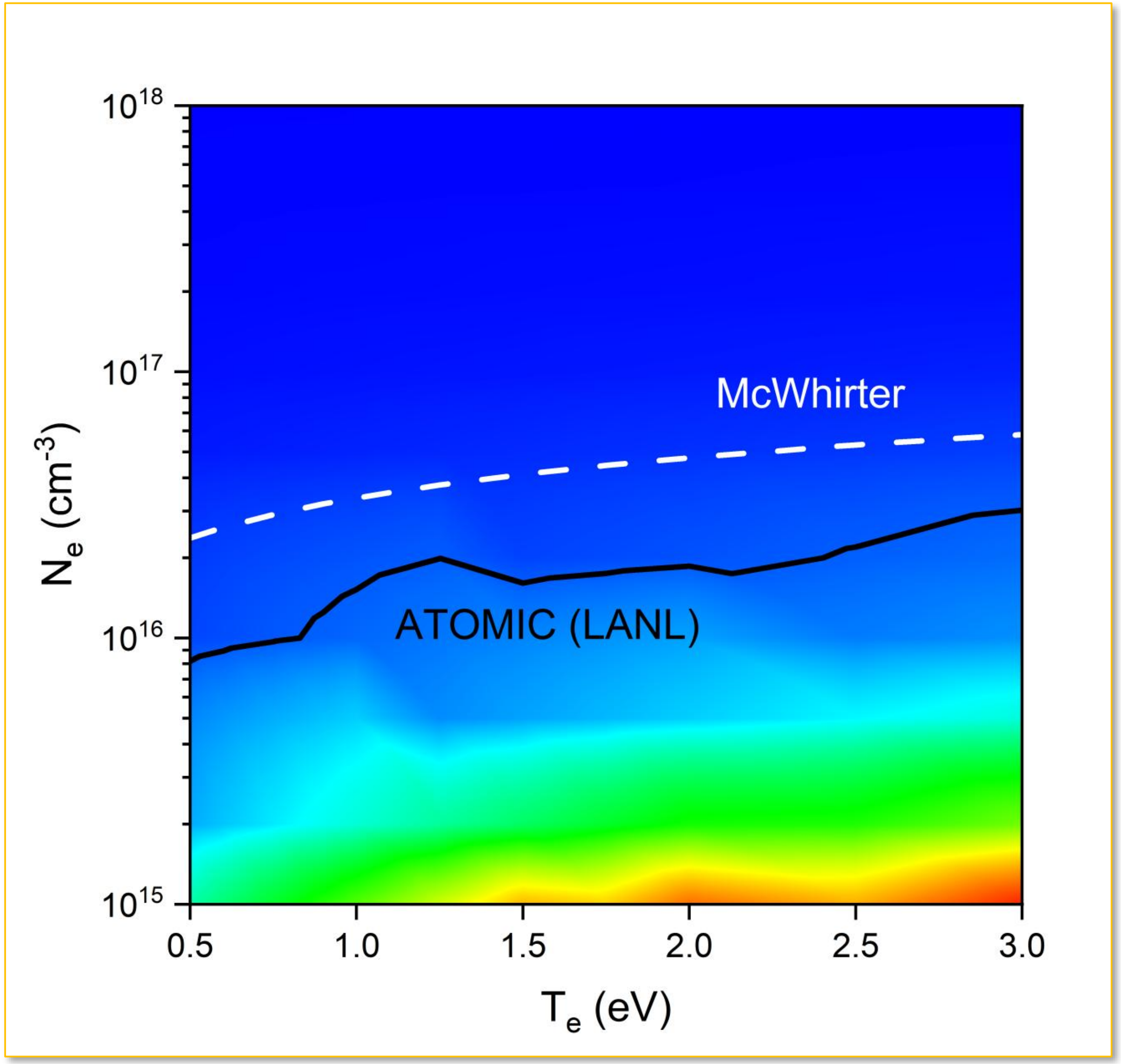
$$\langle\sigma v\rangle_{exc} = \left(\frac{8}{\pi m T^3}\right)^{1/2} \int_{\Delta E}^{\infty} \sigma(E) E e^{-E/T} dE \rightarrow \beta \frac{f_{ij}\bar{g} e^{-\Delta E/T}}{\Delta E \sqrt{T}}$$

$$g_j\langle\sigma v\rangle_{exc} = g_i\langle\sigma v\rangle_{dxc} \cdot e^{-\frac{\Delta E}{T}} \rightarrow \langle\sigma v\rangle_{dxc} = \beta \frac{g_j}{g_i} \frac{f_{ij}\bar{g}}{\Delta E\sqrt{T}}$$

$$A_{ij} = 4.34 \cdot 10^7 \frac{g_j}{g_i} (\Delta E)^2 f_{ji}$$

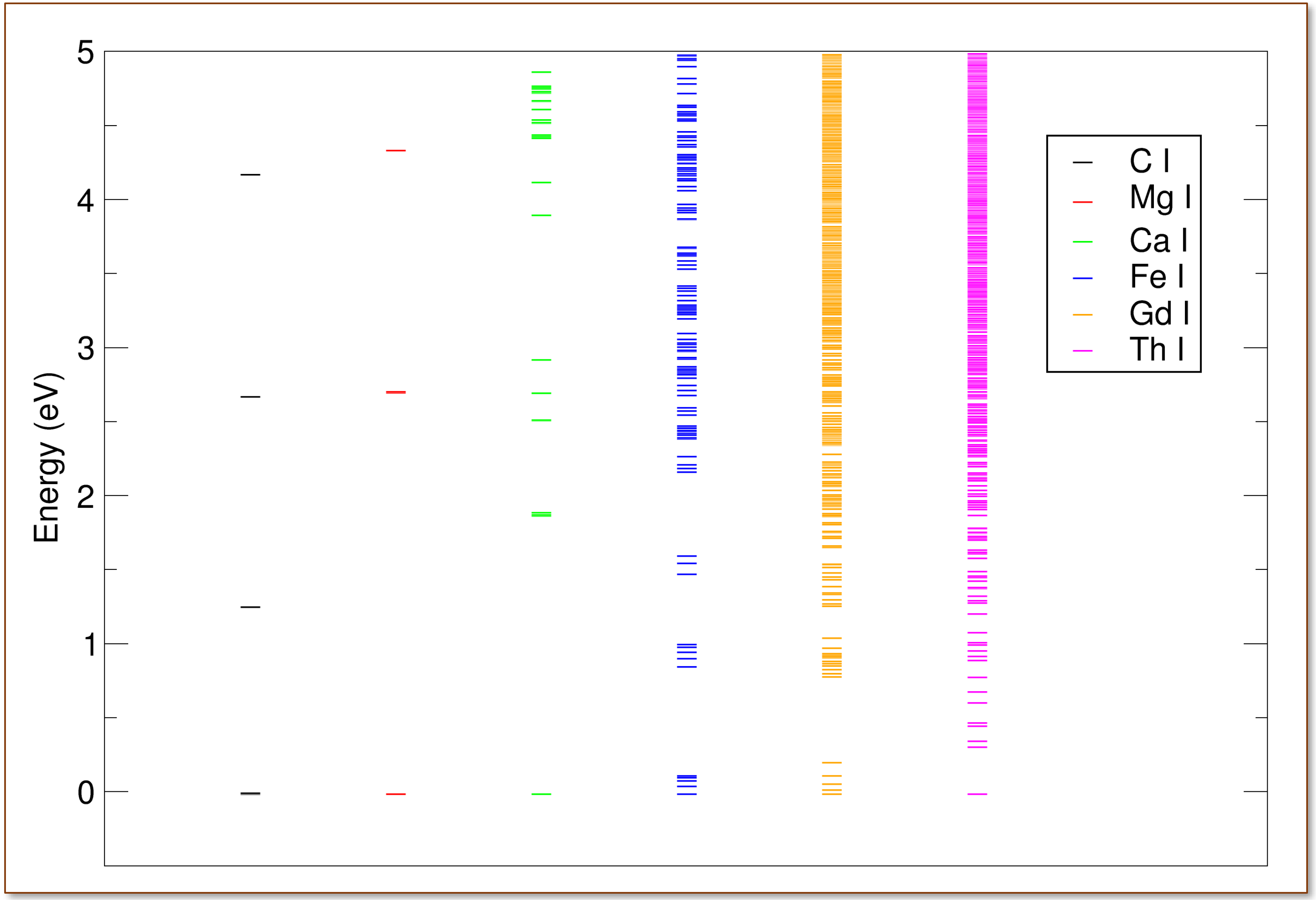
$$n_e \beta \frac{g_j}{g_i} \frac{f_{ij}\bar{g}}{\Delta E\sqrt{T}} > 4.34 \cdot 10^8 \frac{g_j}{g_i} (\Delta E)^2 f_{ji}$$

# Si I



McWhirter
ATOMIC (LANL)
$10^{18}$
$10^{17}$
$10^{16}$
$10^{15}$
$N_e$ (cm$^{-3}$)
0.5
1.0
1.5
2.0
2.5
3.0
$T_e$ (eV)

# *ΔE is very different for different atoms*



# LTE Line Intensities

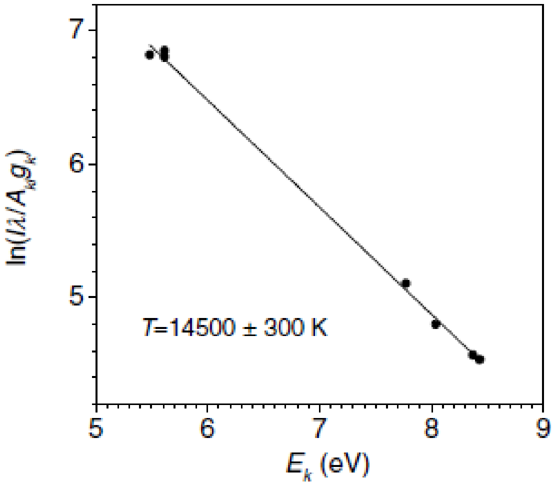
- ***"No" atomic data*** (only *energies* and *statweights*) are needed to calculate populations
- Intensity ratio

$$\frac{I_1}{I_2} = \frac{N_1 \Delta E_1 A_1}{N_2 \Delta E_2 A_2} = \frac{g_1 \Delta E_1 A_1}{g_2 \Delta E_2 A_2} \exp\left(-\frac{E_1 - E_2}{T_e}\right)$$

- Or just plot the intensities on a log scale:

$$I = N \cdot A \cdot E = \frac{g_i}{G} AE \exp(-E_i/T_e)$$

$$\ln(I/g_i AE) = -E_i/T_e - \ln(G)$$




Boltzmann plot

Aragon et al, J Phys B **44**, 055002 (2011)

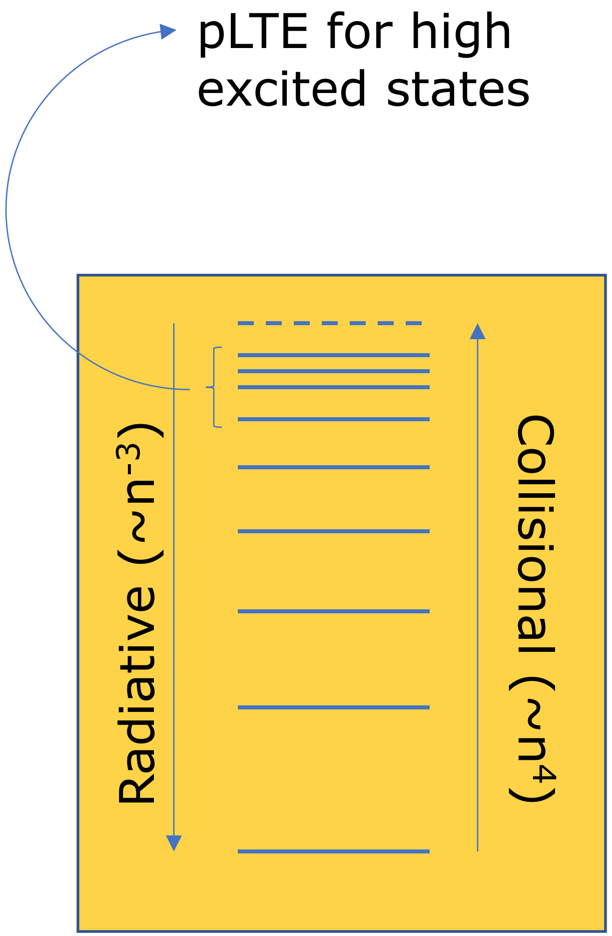
# Saha-LTE conclusions

- Collisions >> radiative processes
  - Saha distribution between ions
  - Boltzmann distribution within ions
- Collisions <u>decrease with Z</u> and radiative processes <u>increase with Z</u>, therefore higher densities are needed for higher ions to reach Saha/LTE conditions
  - H I: $10^{17}$ cm$^{-3}$
  - Ar XVIII: $10^{26}$ cm$^{-3}$

NIST LIBS: can calculate Saha/LTE spectra!!!
(Friday morning)

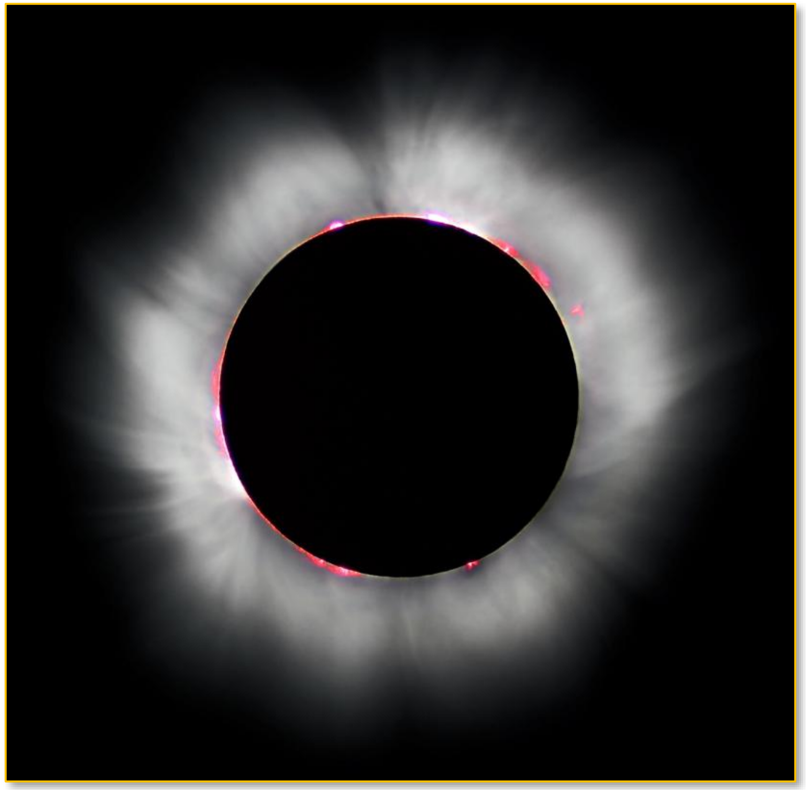
# Deviations from LTE

- Radiative processes are non-negligible
  - LTE: coll.rates ($\sim n_e$) > 10*rad.rates
- Non-Maxwellian plasmas
- Unbalanced processes
- Anisotropy
- External fields
- …

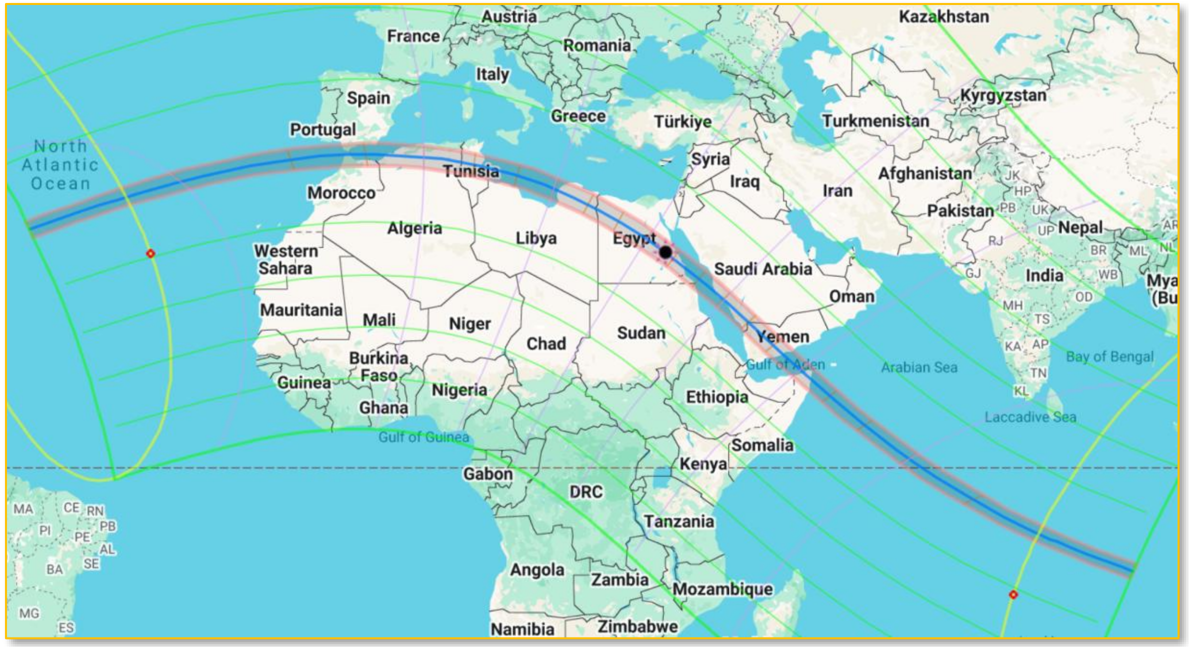


# The other limiting case: Coronal Equilibrium

Low electron densities!



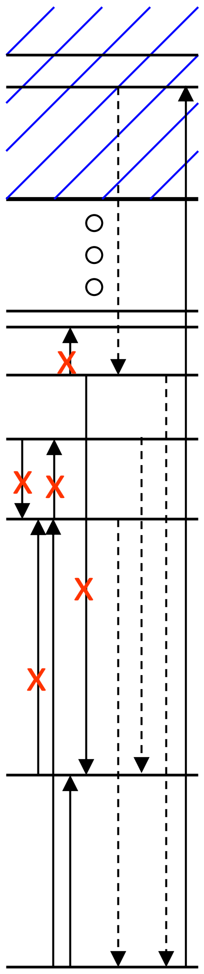
Great SE: Aug 2, 2027



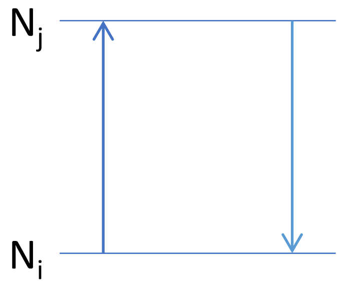

http://xjubier.free.fr/en/site_pages/Solar_Eclipses.html

# Coronal model

- Excitations (and ionization) only from ground state…
- …and metastables
- $A_{rad} \sim n_e^0$, $R_{coll} \sim n_e$ or $n_e^2$
- Does require a complete set of collisional cross sections
- Do we have to calculate all direct and inverse processes?..



# Excitation↔ Deexcitation




Principle of detailed balance: $N_i n_e \langle v\sigma_{ij} \rangle = N_j n_e \langle v\sigma_{ji} \rangle$

In thermodynamic equilibrium:

$$\frac{N_j}{N_i} = \frac{g_j}{g_i} \exp\left(-\frac{\Delta E_{ij}}{T}\right) \quad \Rightarrow \quad g_i \langle v\sigma_{ij} \rangle = g_j \langle v\sigma_{ji} \rangle \exp\left(-\frac{\Delta E_{ij}}{T}\right)$$

Only Maxwell is needed here!

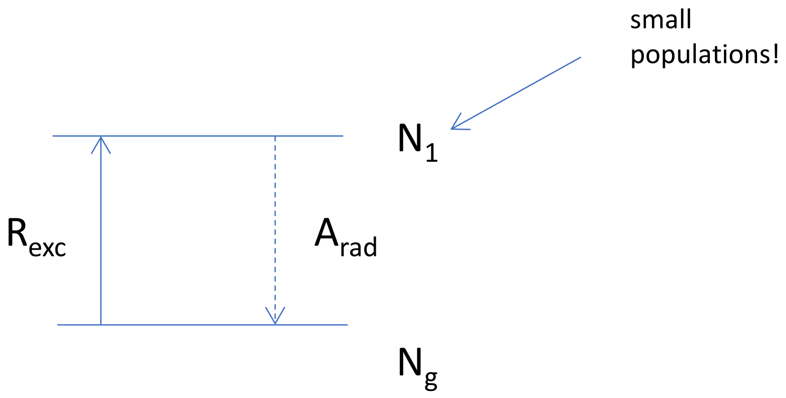
$$g_i \int_{\Delta E}^{\infty} \left(\frac{2E}{m}\right)^{1/2} \sigma_{ij}(E) E^{1/2} e^{-\frac{E}{T}} dE = g_j e^{-\frac{\Delta E}{T}} \int_{0}^{\infty} \left(\frac{2E'}{m}\right)^{1/2} \sigma_{ji}(E') E'^{1/2} e^{-\frac{E'}{T}} dE'$$

Substitution: E ⇒ E+ΔE

$$g_i \int_{0}^{\infty} (E + \Delta E_{ij})\ \sigma_{ij}(\varepsilon + \Delta E)\ e^{-\frac{E}{T}} dE = g_j \int_{0}^{\infty} E\ \ \sigma_{ji}(E)\ e^{-\frac{E}{T}} dE$$

Must be valid for any T, therefore: $g_i (E + \Delta E) \sigma_{ij}^{exc}(E + \Delta E) = g_j E \sigma_{ij}^{dxc}(E)$

# Line Intensities under CE (no TD)




Balance equation:

$$N_g R_{exc} = N_1 A_{rad}$$

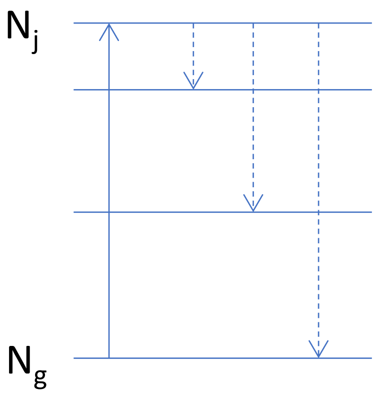
$$N_1 = \frac{N_g R_{exc}}{A_{rad}} = \frac{N_g n_e \langle v\sigma \rangle}{A_{rad}}$$

$$I = N_1 A_{rad} E = N_g R_{exc} E$$

**Line intensity does NOT depend on $A_{rad}$!**

$I \propto n_e$

If more than one radiative transition:




$$N_g R_{exc} = N_j \sum_{i<j} A_{ij}$$

$$N_j = \frac{N_g R_{exc}}{\sum_{i<j} A_{ij}} = \frac{N_g n_e \langle v\sigma_{jg} \rangle}{\sum_{i<j} A_{ij}}$$

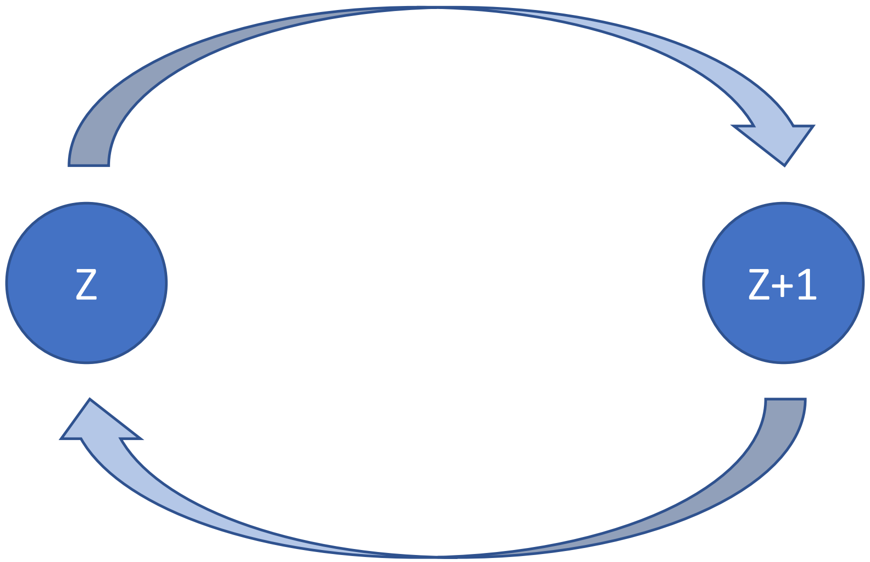
$$I_{ij} = N_j E_{ij} A_{ij}$$

$$= N_g n_e \langle v\sigma_{jg} \rangle \frac{A_{ij}}{\sum_{k<j} A_{kj}}$$

Cascades may be important

# Ionization Balance in CE

Electron-impact ionization: $\propto n_e$




Photorecombination and DR: $\propto n_e$

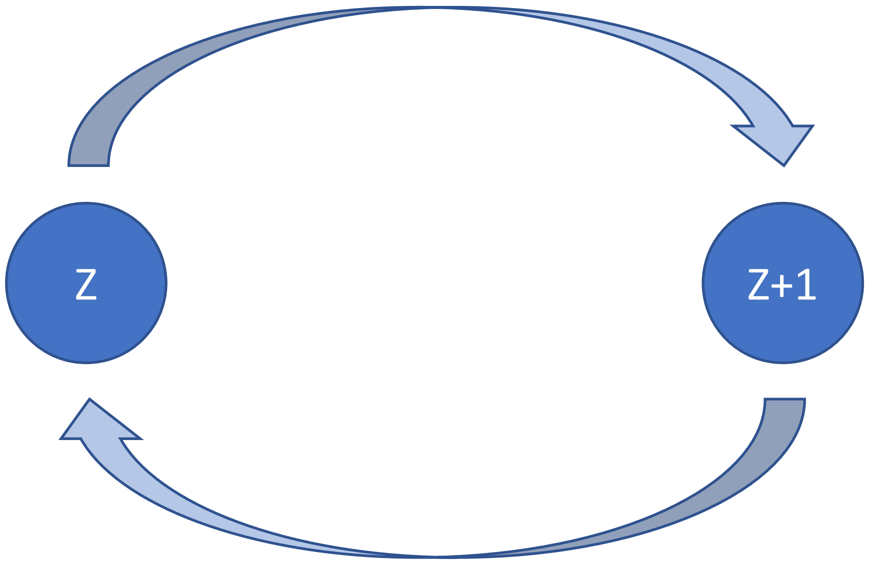
$$\frac{N_{Z+1}}{N_Z} = \frac{n_e\langle v\sigma\rangle_{ion}}{n_e\langle v\sigma\rangle_{RR} + n_e\langle v\sigma\rangle_{DR}}$$

Independent of $n_e$!

Most abundant ion: $\frac{I_Z}{T_e} \sim 3 \ (Z_N < 30)$

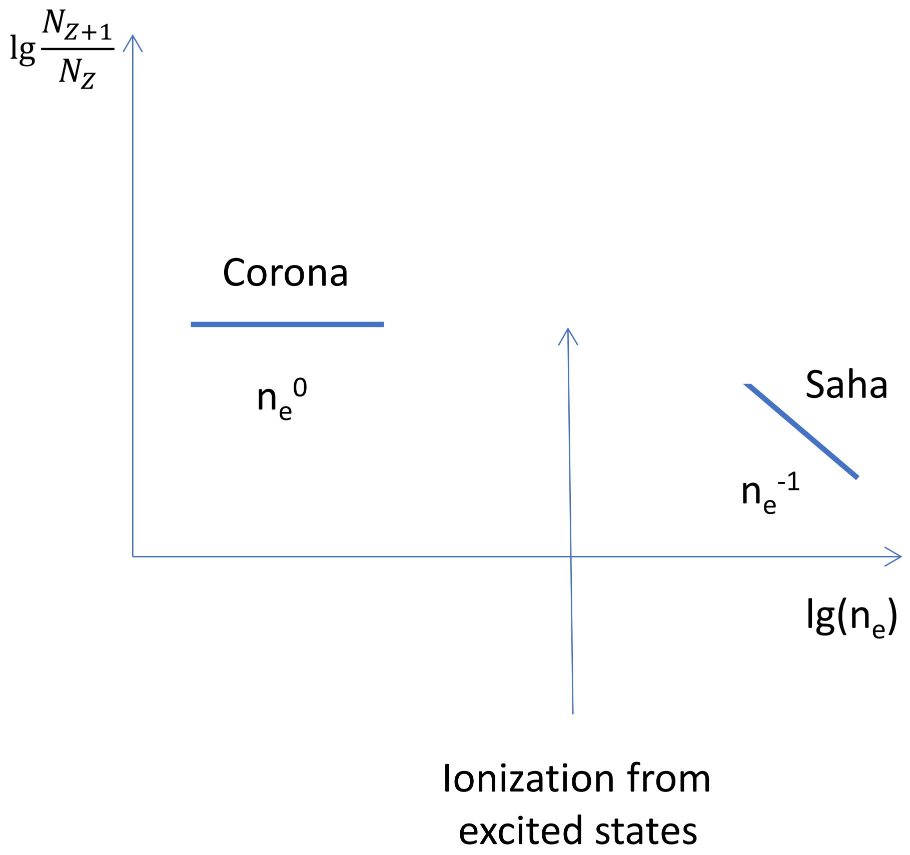
# Ionization Balance in a General Case

Electron-impact ionization: $\propto n_e$

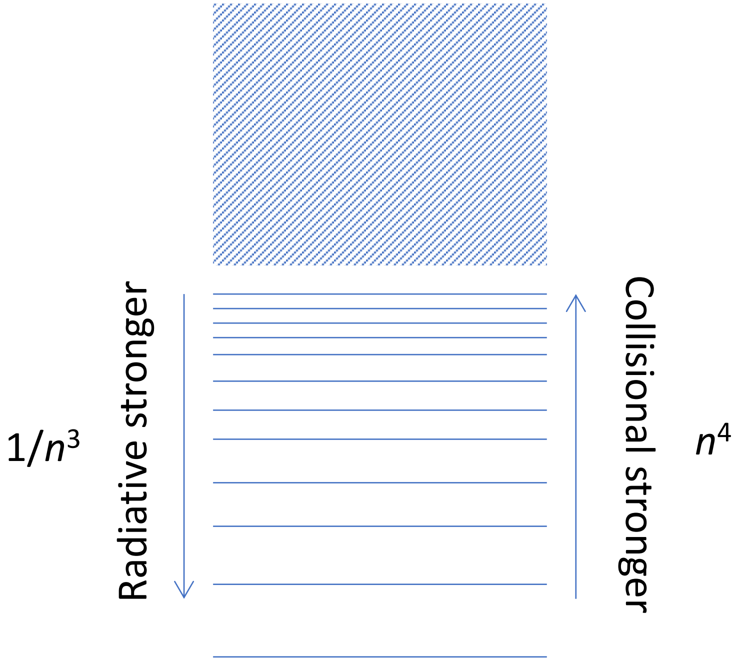


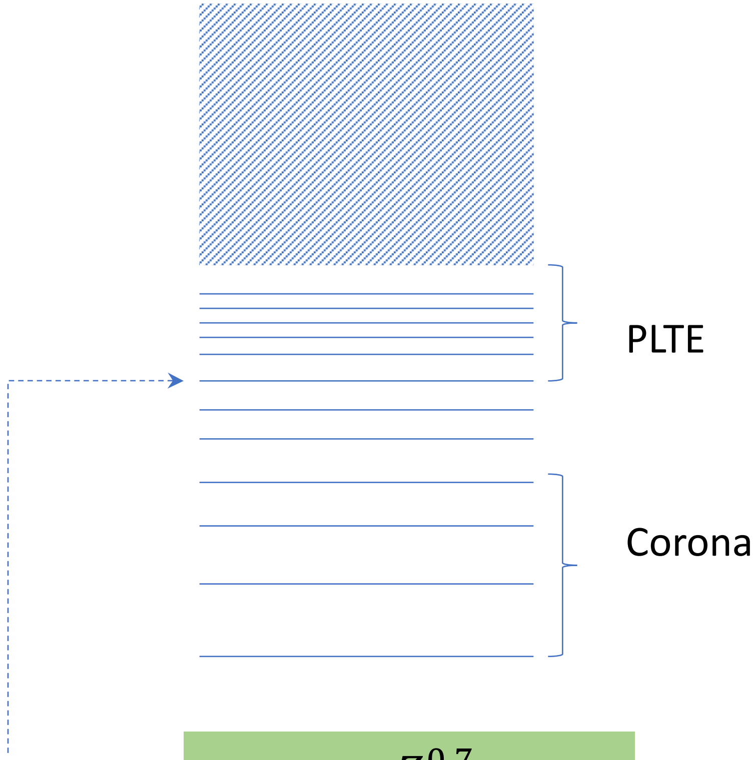

Photorecombination and DR: $\propto n_e$

3-body recombination: $\propto n_e^2$



# From Corona to PLTE

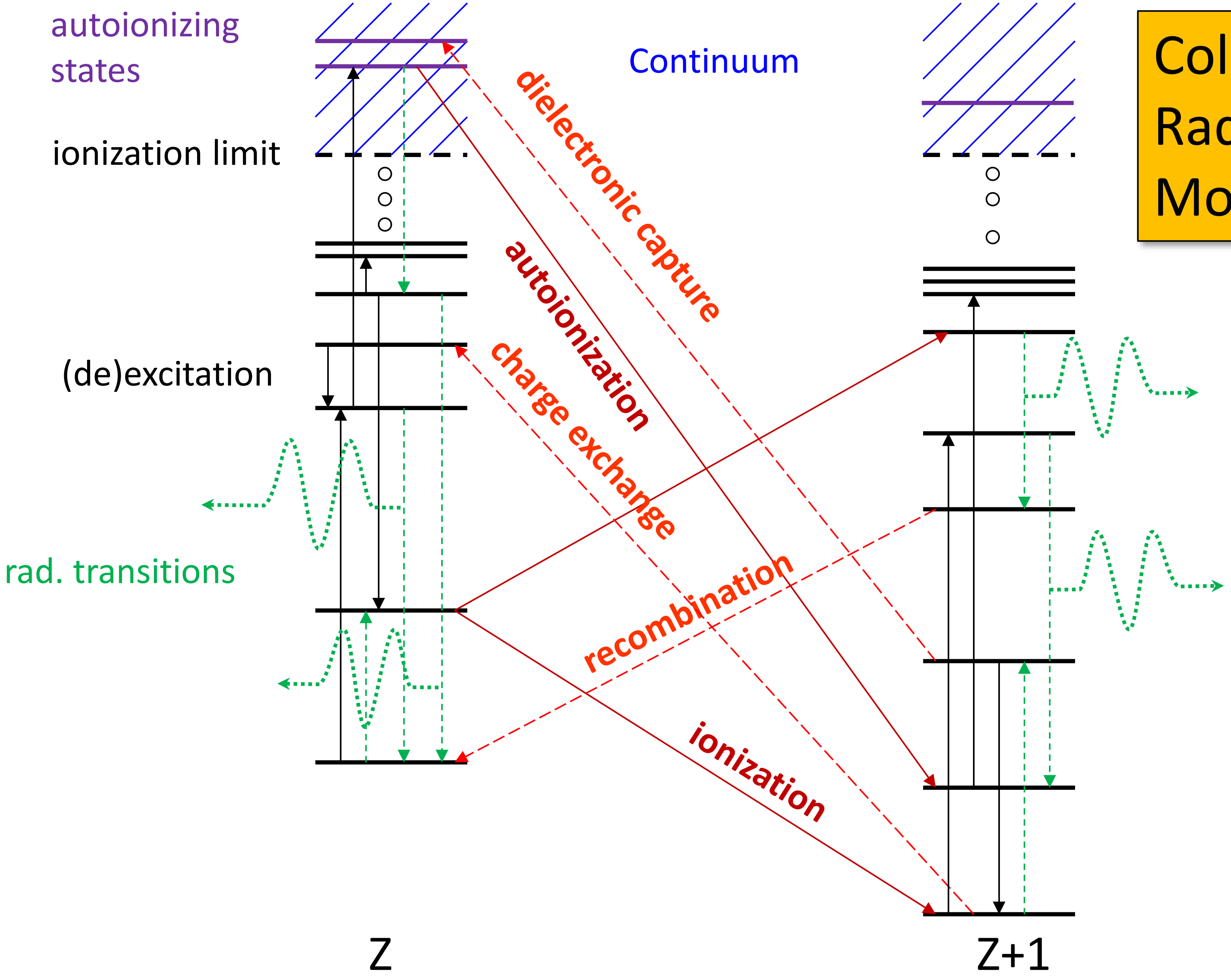



Griem limit: $$n \sim 140 \cdot \frac{Z^{0.7}}{n_e^{2/17}} T_e^{1/17}$$

$n_e = 10^{18}$ cm$^{-3}$, $T_e = 100$ eV, $Z = 10$: ***n=7***

# Collisional-Radiative Model



# Basic rate equation

$$\hat{N} = \begin{pmatrix} \cdots \\ N_{Z,i} \\ \cdots \end{pmatrix}$$

Vector of atomic states populations

$$\frac{d\hat{N}(t)}{dt} = \hat{A}\big(t, \hat{N}(t), n_e, n_i, T_e, T_i \ldots\big) \cdot \hat{N}(t) + \hat{S}(t)$$

Rate matrix

Source function

**Off-diagonal**: total rates of all processes between two levels
**Diagonal**: total destruction rates for a level

# Basic rate equation (cont'd)

$$\frac{dN_{Zi}}{dt} = \sum_{j<i} N_{Z,j}\left(R_{Z,ji}^{e-exc} + R_{Z,ji}^{h-exc} + B_{Z,ji}^{p-exc}\right)$$
$$+ \sum_{j>i} N_{Z,j}\left(R_{Z,ji}^{e-dexc} + R_{Z,ji}^{h-dexc} + A_{Z,ji}^{sp-rad} + B_{Z,ji}^{st-rad}\right)$$
$$+ \sum_{Z'>Z} \sum_{k\in Z'} N_{Z',k}\left(\alpha_{Z'k,Zi}^{3b} + \alpha_{Z'k,Zi}^{rr} + \alpha_{Z'k,Zi}^{dc} + \alpha_{Z'k,Zi}^{cx}\right)$$
$$+ \sum_{Z'<Z} \sum_{k\in Z'} N_{Z',k}\left(S_{Z'k,Zi}^{e-ion} + S_{Z'k,Zi}^{i-ion} + S_{Z'k,Zi}^{p-ion} + S_{Z'k,Zi}^{cx}\right)$$

Population influx

$$-N_{Z,i} \times$$
$$\left(\sum_{j>i}\left(R_{Z,ij}^{e-exc} + R_{Z,ij}^{h-exc} + B_{Z,ij}^{p-exc}\right)\right.$$
$$+ \sum_{j<i}\left(R_{Z,ji}^{e-dexc} + R_{Z,ji}^{h-dexc} + A_{Z,ji}^{sp-rad} + B_{Z,ji}^{st-rad}\right)$$
$$+ \sum_{Z'<Z} \sum_{k\in Z'}\left(\alpha_{Zi,Z'k}^{3b} + \alpha_{Zi,Z'k}^{rr} + \alpha_{Zi,Z'k}^{dc} + \alpha_{Zi,Z'k}^{cx}\right)$$
$$\left. + \sum_{Z'<Z} \sum_{k\in Z'}\left(S_{Zi,Z'k}^{e-ion} + S_{Zi,Z'k}^{i-ion} + S_{Zi,Z'k}^{p-ion} + S_{Zi,Z'k}^{cx}\right)\right)$$
$$+S_i$$

Population outflux

# CR model: features

1. Most general approach to population kinetics
2. Depends on detailed atomic data and requires a lot of them…
3. Should reach Saha/LTE conditions at high densities and coronal at low
4. May include from tens to millions of atomic states

*CRETIN* *DLAZY*

*FLYCHK* *PRISMSPEC*

*SCRAM*

*AVERROES*

*ATOMIC* *CRAC* …

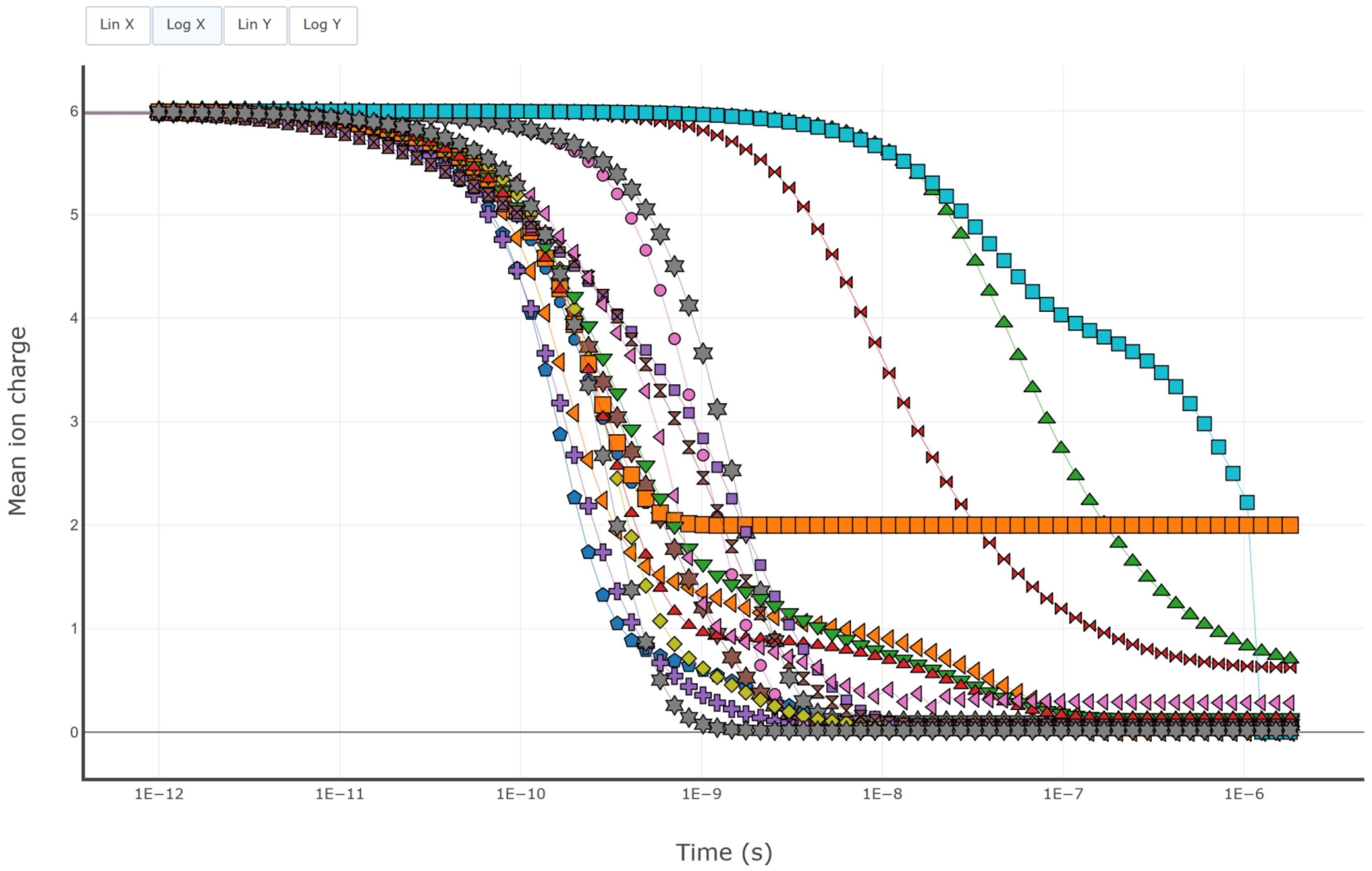
*NOMAD*

# CR model: questions to ask

1. What state description is relevant?
2. What are the most (and not so) important physical processes?
3. How to calculate the rates? What is the source of the data?
4. Which level of data accuracy is sufficient for this particular problem?
5. Which plasma effects are important? Opacity? IPD?

There is NO universal CR model for all cases

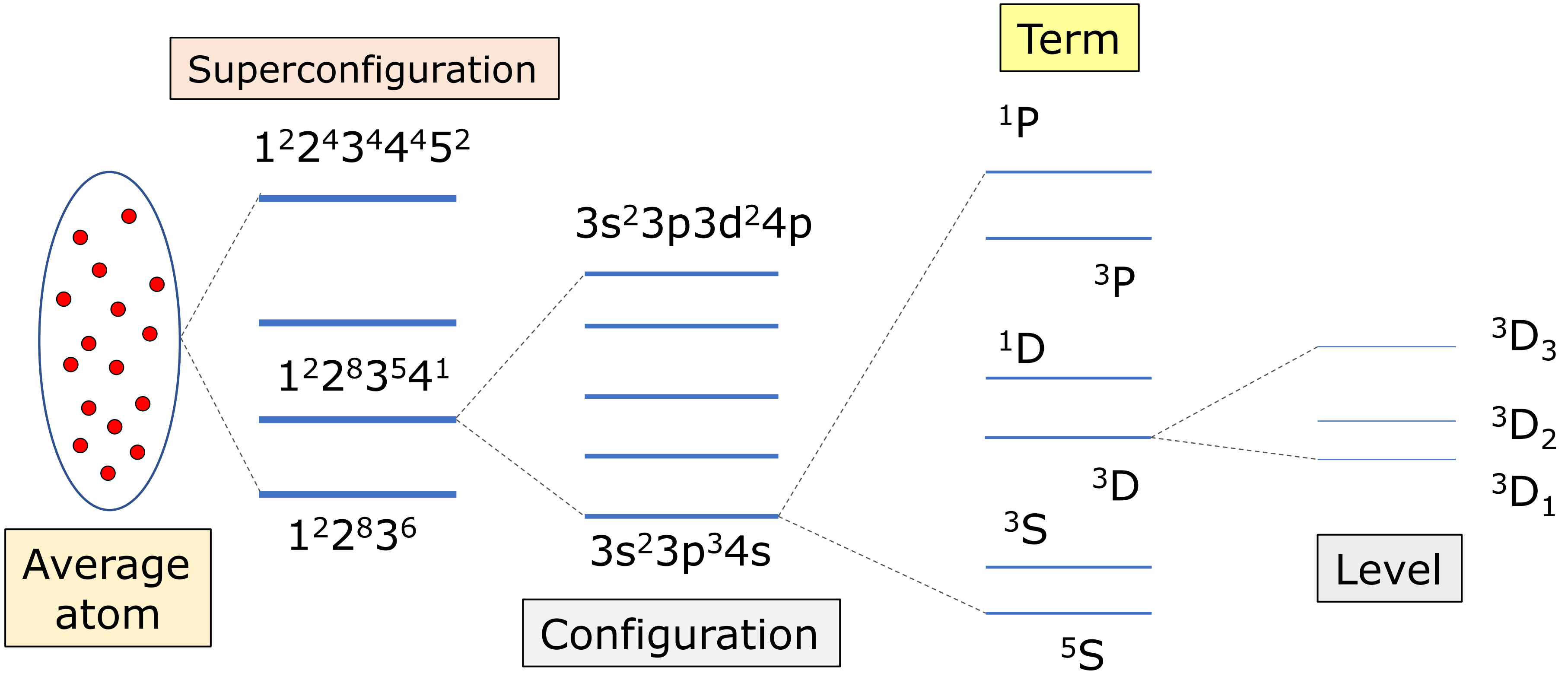
# CR models: validation and verification




**NLTE-13**

Recombination of fully stripped carbon at 1 eV

# 16-electron ion (S-like)

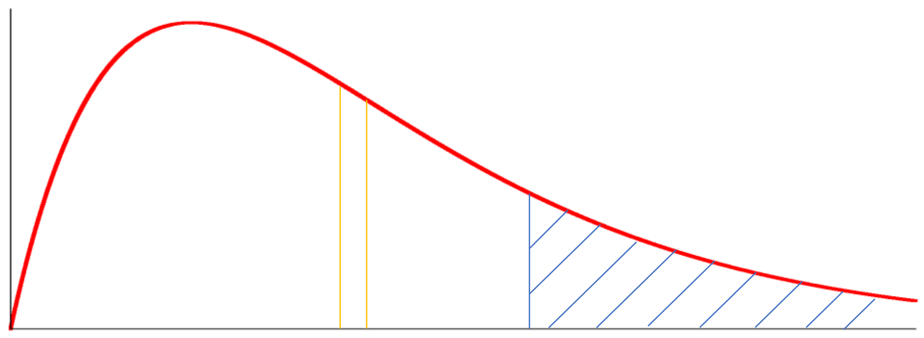



Even parabolic states for motional Stark effect!

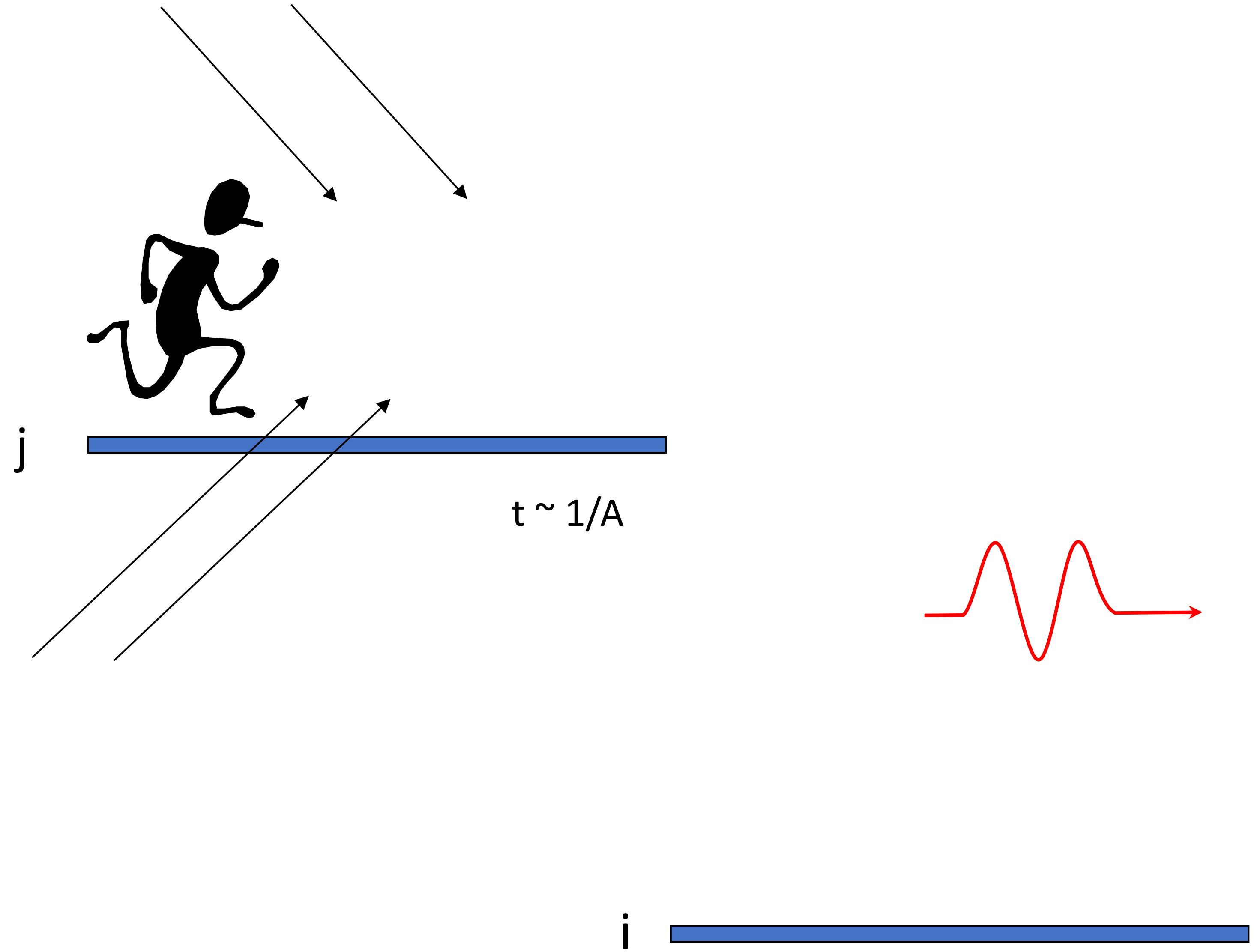
# Some principles for line intensity ratio diagnostics

- Electron density
  - Collisional dumping (density-dependent outflux)
  - Density-dependent influx

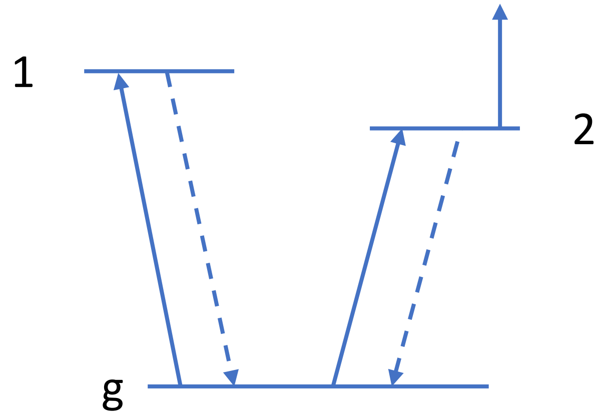
- Electron temperature
  - Different parts of Maxwellian populate different lines (upper levels)



# Why are the forbidden lines sensitive to density?



# Let put him into a formula:




Strong transition

$$N_g n_e \langle \sigma v \rangle_{g1} = N_1 A_1$$

$$N_g n_e \langle \sigma v \rangle_{g2} = N_2 A_2 + N_2 n_e \langle \sigma v \rangle_2$$

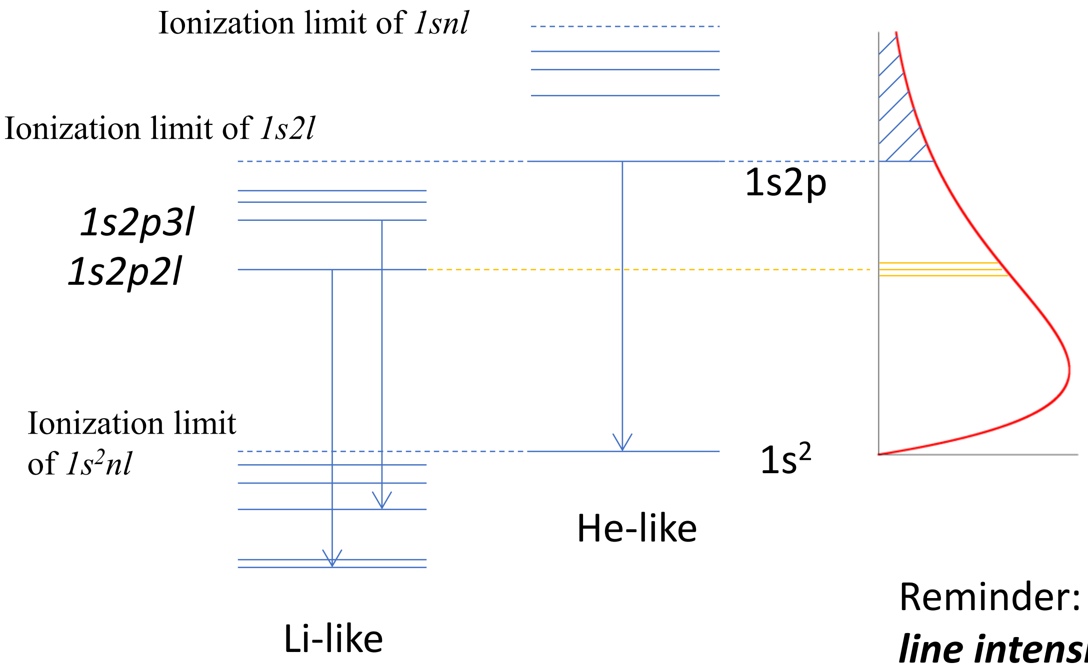
$$N_1 = \frac{N_g n_e \langle \sigma v \rangle_{g1}}{A_1}$$

$$N_2 = \frac{N_g n_e \langle \sigma v \rangle_{g2}}{A_2 + n_e \langle \sigma v \rangle_2}$$

$$\frac{N_1 A_1}{N_2 A_2} = \frac{\langle \sigma v \rangle_{g1}}{\langle \sigma v \rangle_{g2}} \cdot \frac{A_2 + n_e \langle \sigma v \rangle_2}{A_1}$$

E.g., resonance to intercombination lines in He-like ions

# Temperature diagnostics with DS




Excitation rate for *1s2p* ~ $\frac{e^{-\frac{E_W}{T}}}{T^{1/2}}$

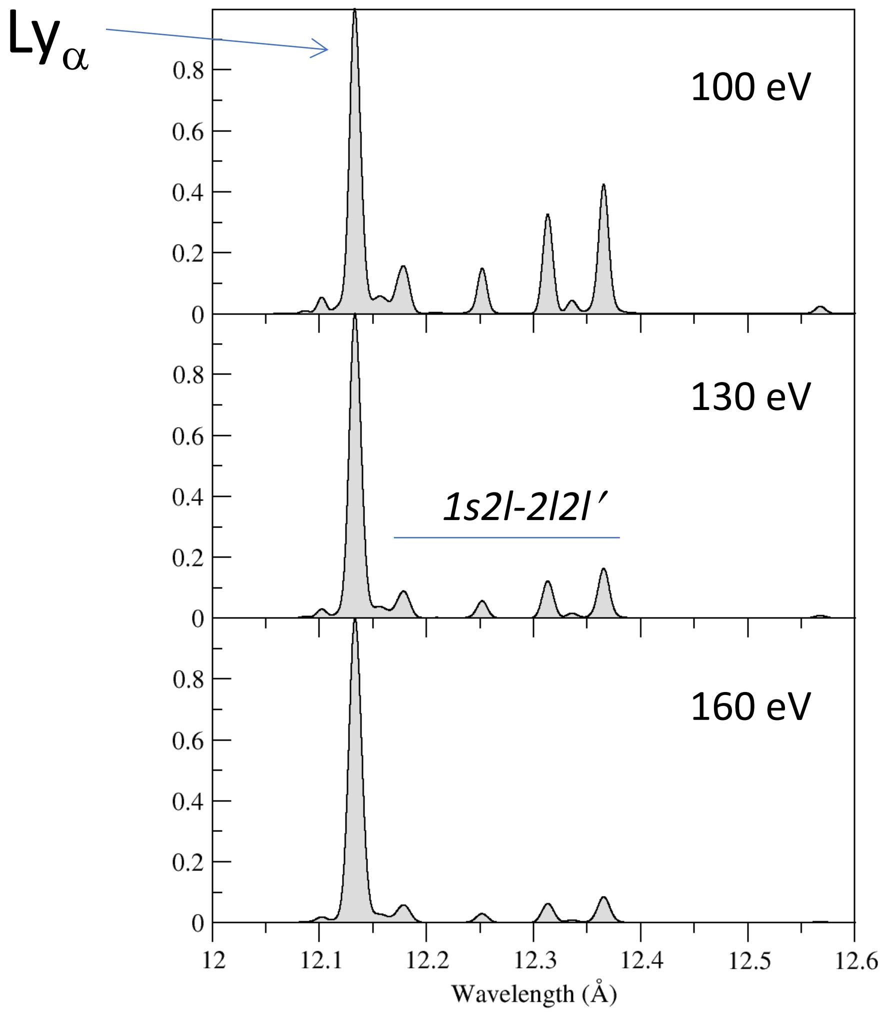
DC rate for *1s2l2l′*~ $\frac{e^{-\frac{E_S}{T}}}{T^{3/2}}$

Reminder: for (low-density) coronal conditions
***line intensity = population influx***

Therefore: $$\frac{I_S}{I_W} \propto \frac{\exp\left(-\frac{\Delta E}{T}\right)}{T} \sim \frac{1}{T}$$

Independent of ionization balance since the initial state is the same!

# Temperature dependence: $Ly_\alpha$ satellites



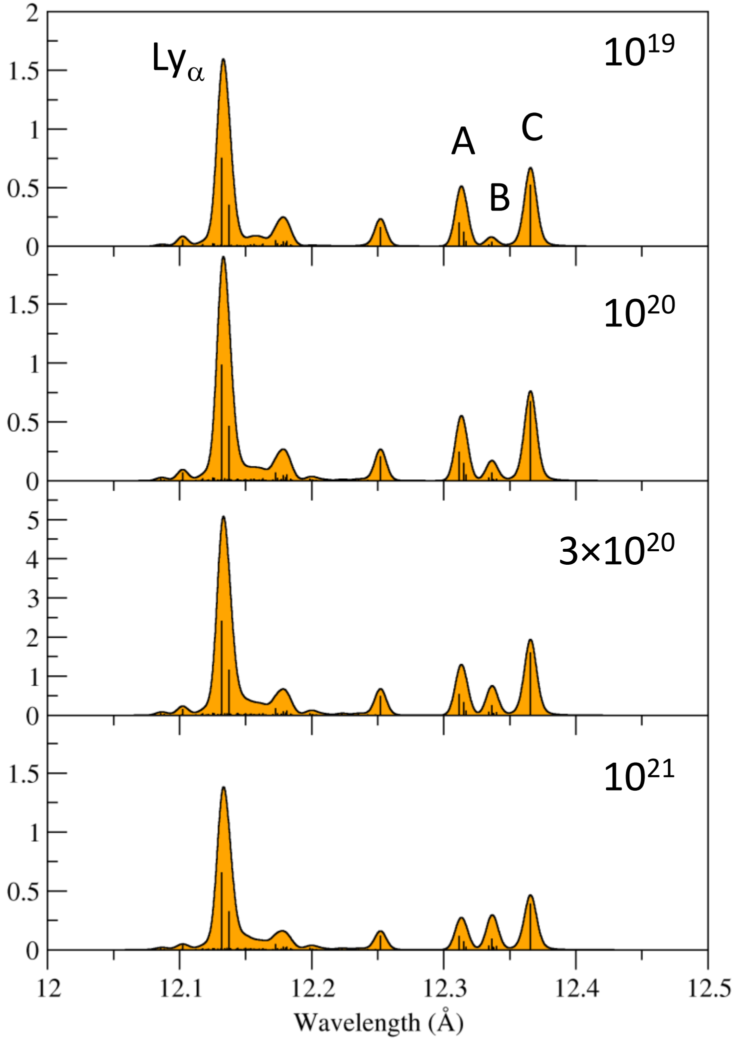

H-like Ne X

$1s_{1/2}$-$2p_{1/2}$

$1s_{1/2}$-$2p_{3/2}$

*1snl-2l′nl*, n=2,3,4,…

# Density diagnostics with DS

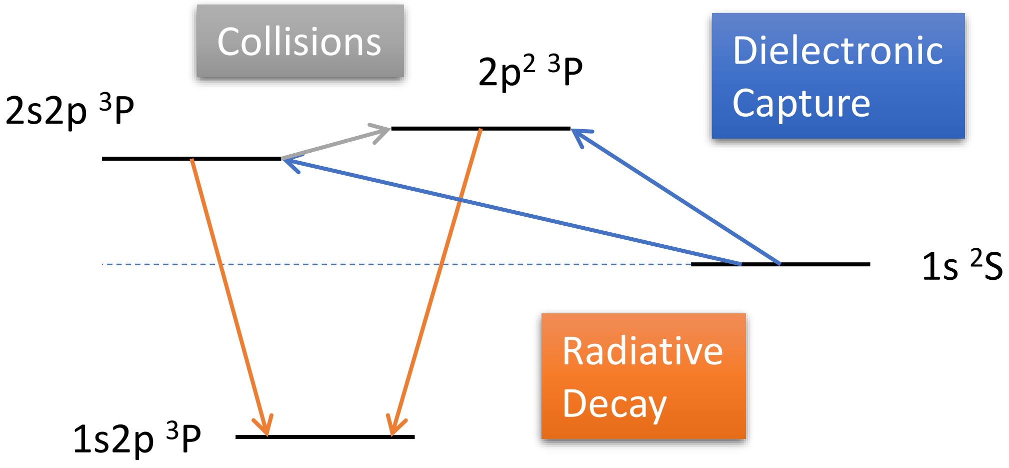



Ne X $Ly_\alpha$ and satellites *1snl-2pnl*

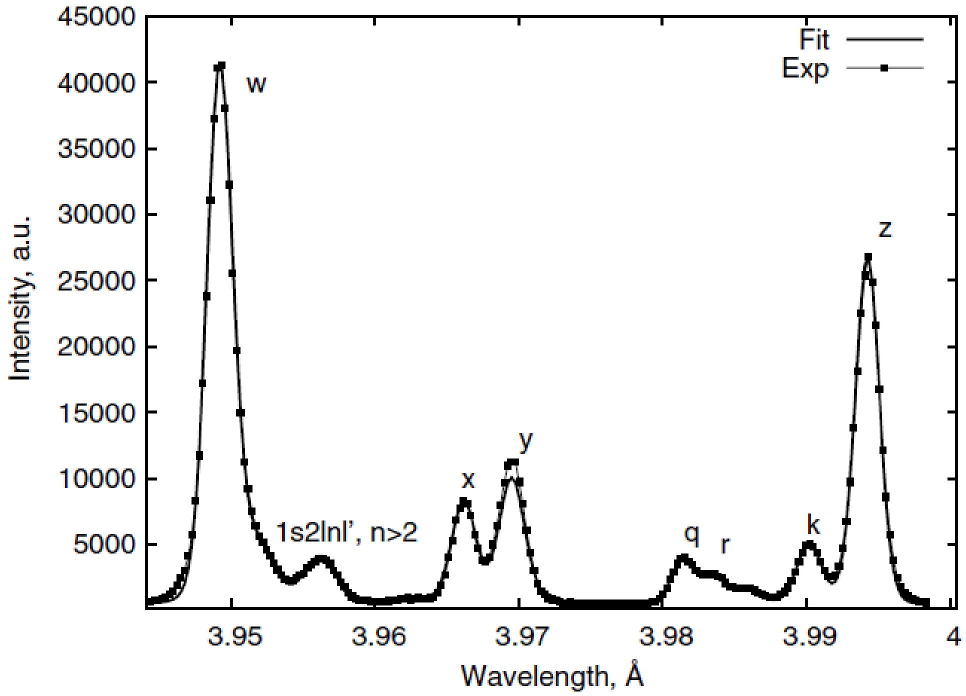
A. $1s2s\ ^3S_1 - 2s2p\ ^3P_{0,1,2}$

B. $1s2p\ ^3P_{0,1,2} - 2p^2\ ^3P_{0,1,2}$

C. $1s2p\ ^1P_1 - 2p^2\ ^1D_2$ (J satellite)



# He-like lines and satellites

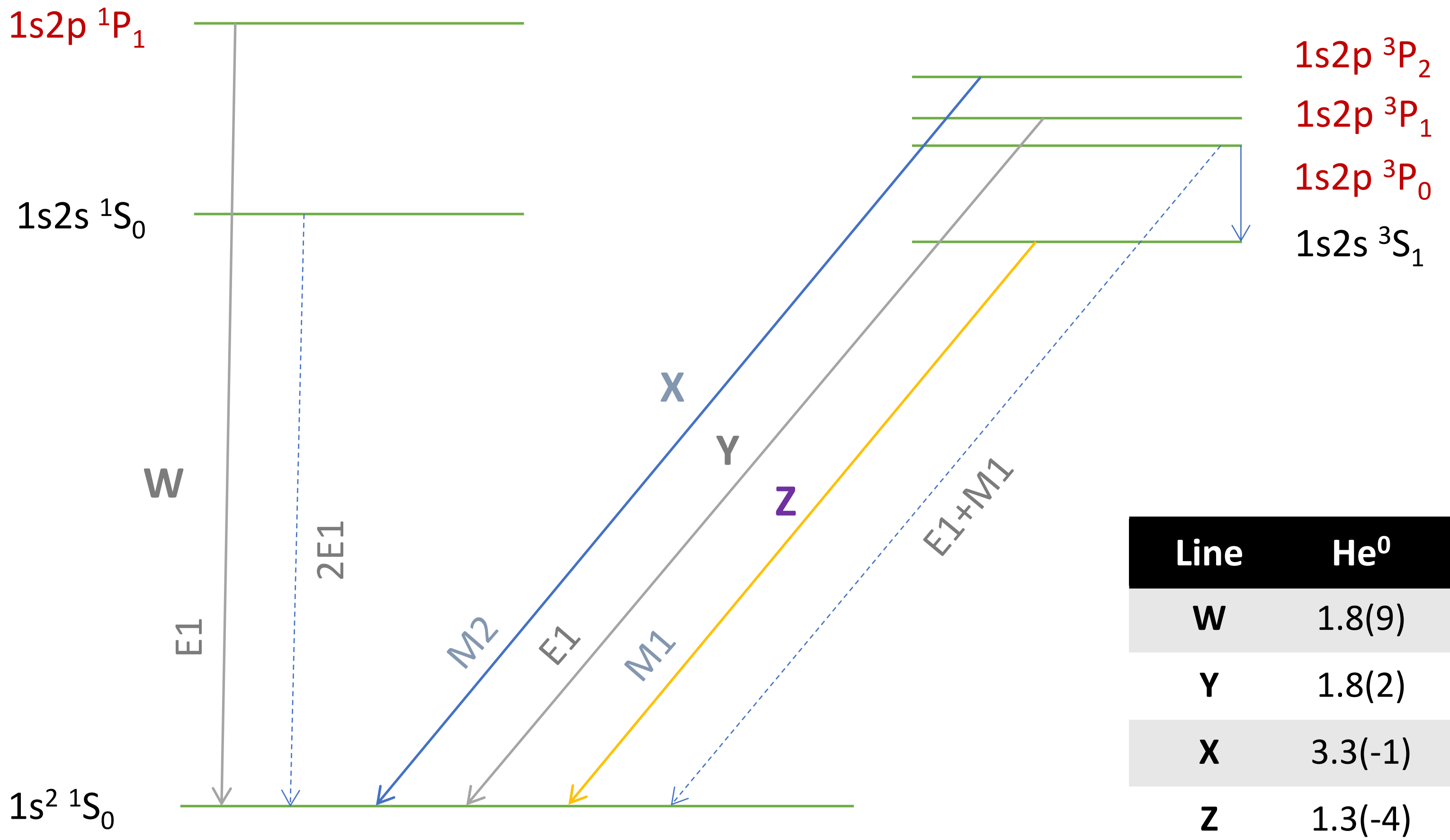



O.Marchuk et al, J Phys B 40, 4403 (2007)

# Energy levels in He-like Ar

- Ground state: $1s^2\ {}^1S_0$
- Two subsystems of terms
  - Singlets **1*snl*** $^1$**L**, J=*l* (example $1s3d\ {}^1D_2$)
  - Triplets **1*snl*** $^3$**L**, 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

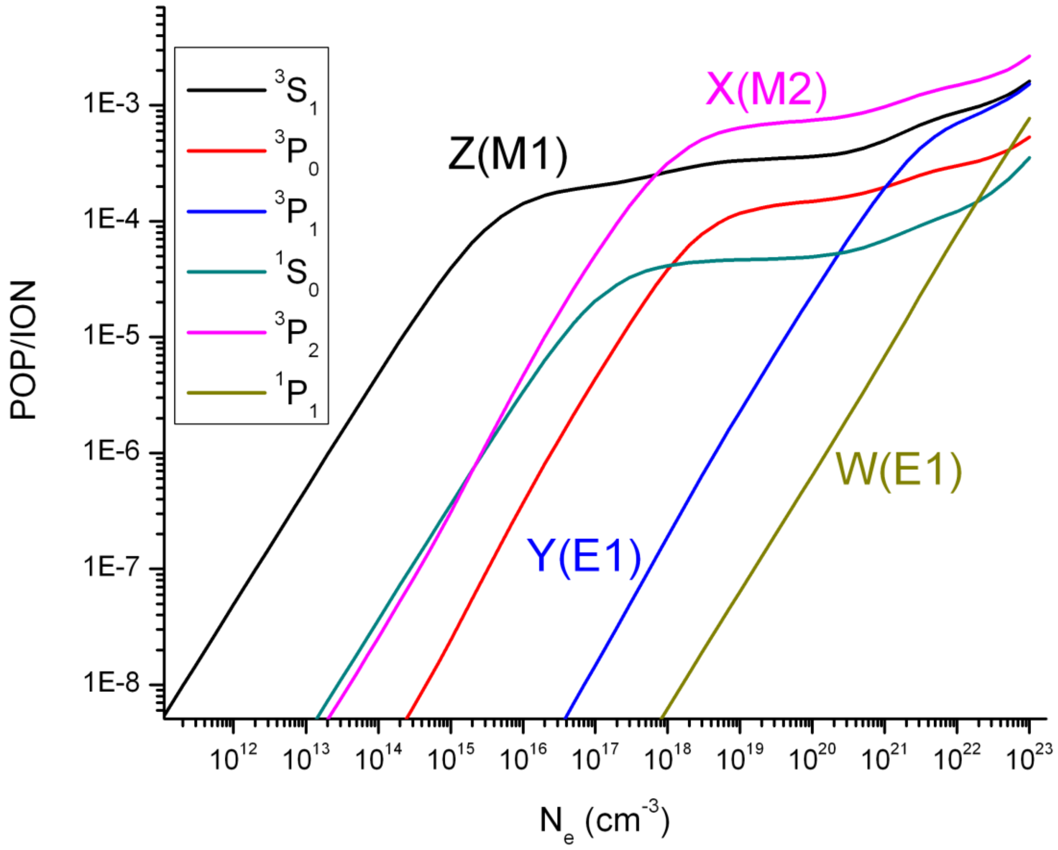



| Line | $He^0$ | $Ar^{16+}$ | $Fe^{25+}$ | $Kr^{34+}$ |
|---|---|---|---|---|
| W | 1.8(9) | 1.1(14) | 4.6(14) | 1.5(15) |
| Y | 1.8(2) | 1.8(12) | 4.4(13) | 3.9(14) |
| X | 3.3(-1) | 3.1(8) | 6.5(9) | 9.3(10) |
| Z | 1.3(-4) | 4.8(6) | 2.1(8) | 5.8(9) |

# 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]: $A(1s^2\ ^1S_0 - 1s2s\ ^3S_1) \propto \mathbf{Z^{10}}$

# n=2 populations



# Ar XVII Line Ratios