Atomic Data for Plasmas:
Line Intensities and CR Modeling

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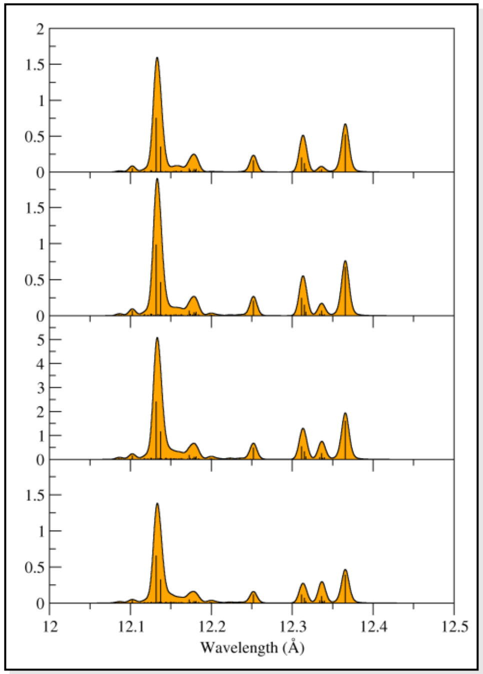

Joint ICTP-IAEA School on Data for Modelling Atomic and Molecular Processes in Plasmas
Match 18-22 2024, ICTP, Trieste, Italy

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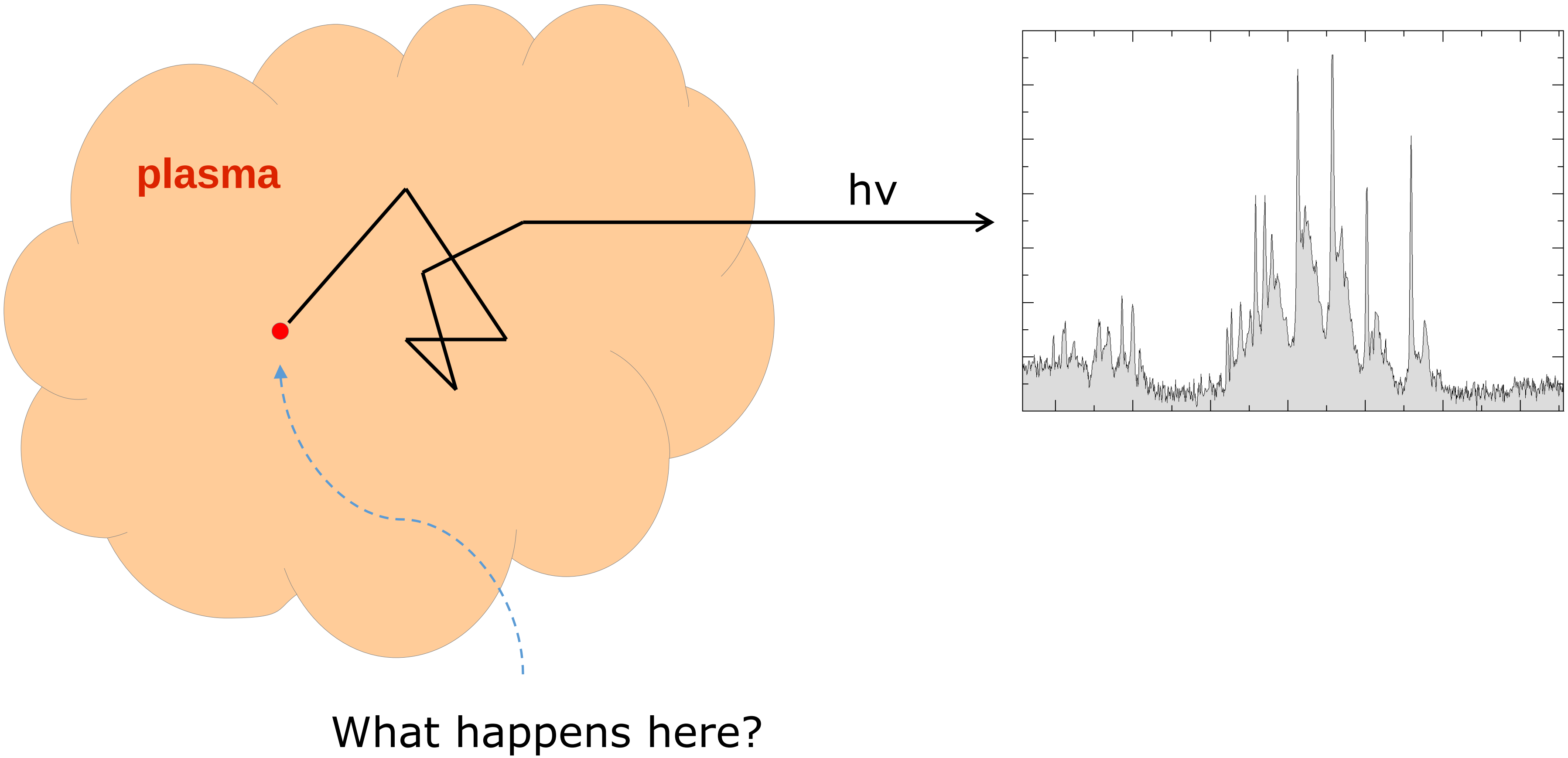

plasma
hν
What happens here?

Example: Spectral Line Intensity (thin)

Upper state density (cm^{-3})

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

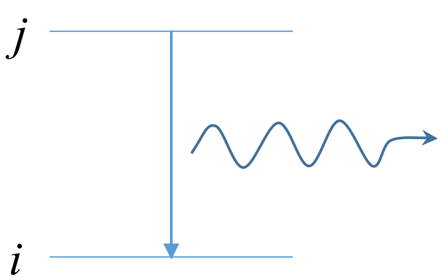
strongly depends on plasma conditions

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

(*almost*) purely atomic parameters

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

Photon energy (eV)



Scaling reminder:

Radiation

$A_r(Z_c=1,E1) \sim \mathbf{10^8}\ s^{-1}$; $A_r(Z_c=1,M1/E2) \sim \mathbf{1}\ s^{-1}$

$A_r(E1) \sim \mathbf{Z^4}$; $A_r(\text{forbidden}) \sim \mathbf{Z^6\text{-}Z^{12}}$

Autoionization

$A_a(E1) \sim \mathbf{10^{13}\text{-}10^{14}}\ s^{-1}$

Collisions

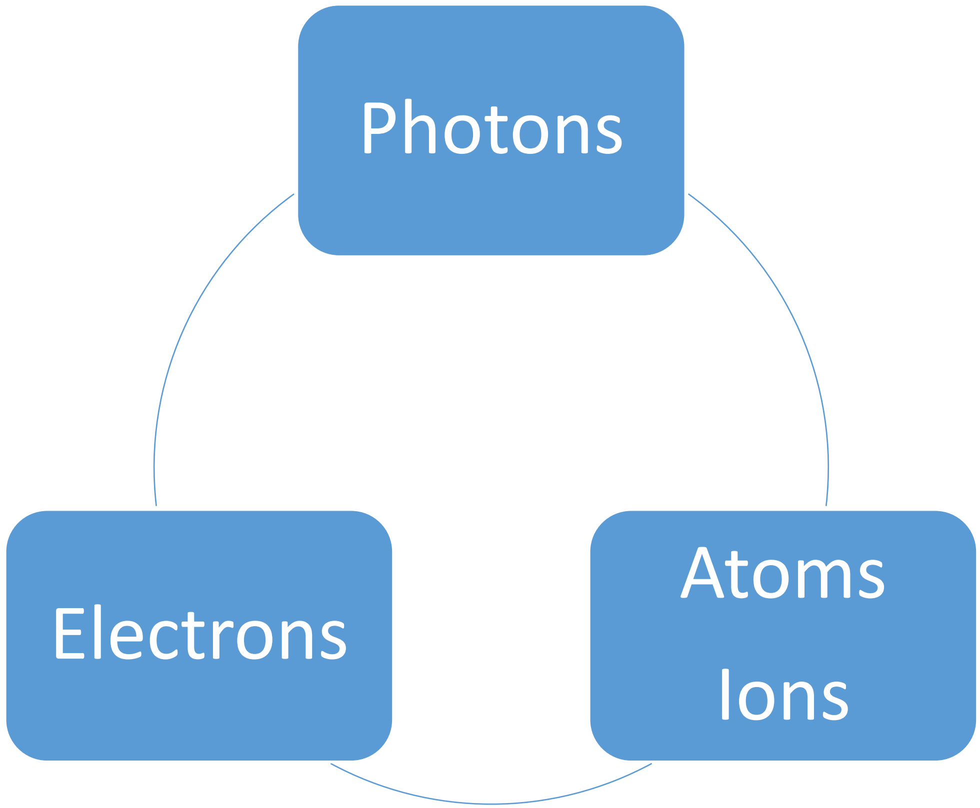
$\sigma(Z_c=1) \sim \mathbf{10^{-16}}\ cm^2$; $\langle\sigma v\rangle \sim \mathbf{10^{-8}}\ cm^3/s$

$\sigma \sim \mathbf{Z^{-3}\text{–}Z^{-4}}$; $\langle\sigma v\rangle \sim \mathbf{Z^{-2}\text{-}Z^{-3}}$

Thermodynamic equilibrium

Principle of detailed balance

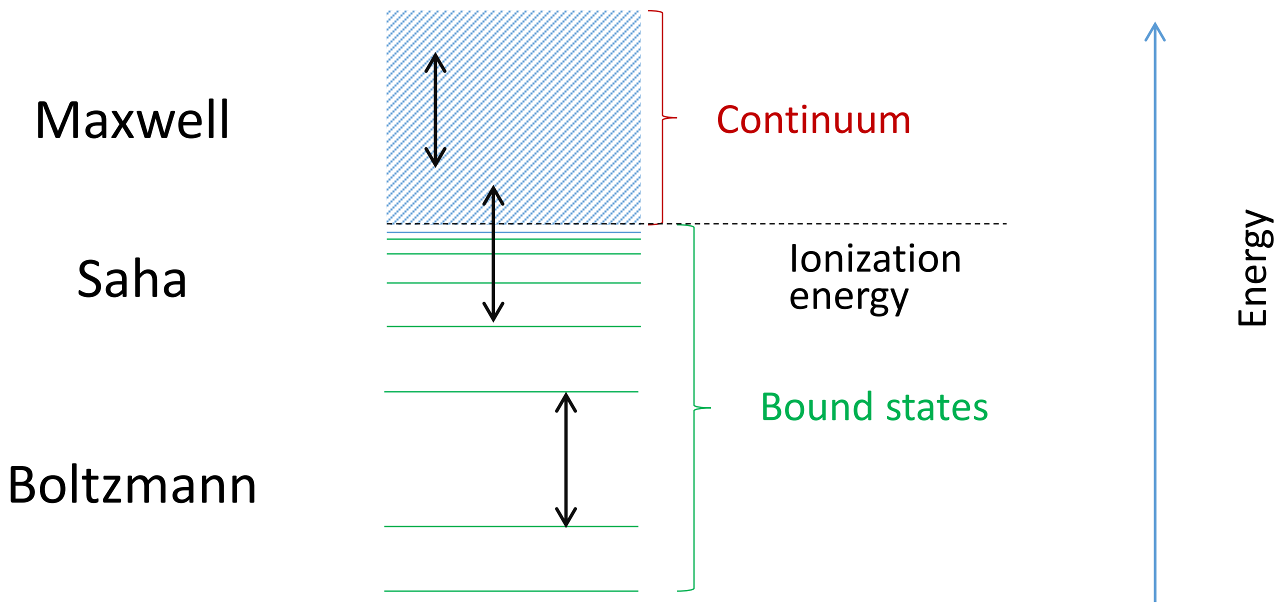
- ***each direct process is balanced by the inverse***
  - excitation ↔ deexcitation
  - ionization ↔ 3-body recombination
  - photoionization ↔ photorecombination
  - autoionization ↔ dielectronic capture
  - radiative decay (spontaneous+stimulated) ↔ photoexcitation



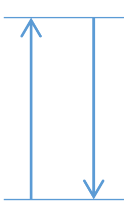
TE: distributions

- 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

Thermodynamic equilibrium: energy scheme



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



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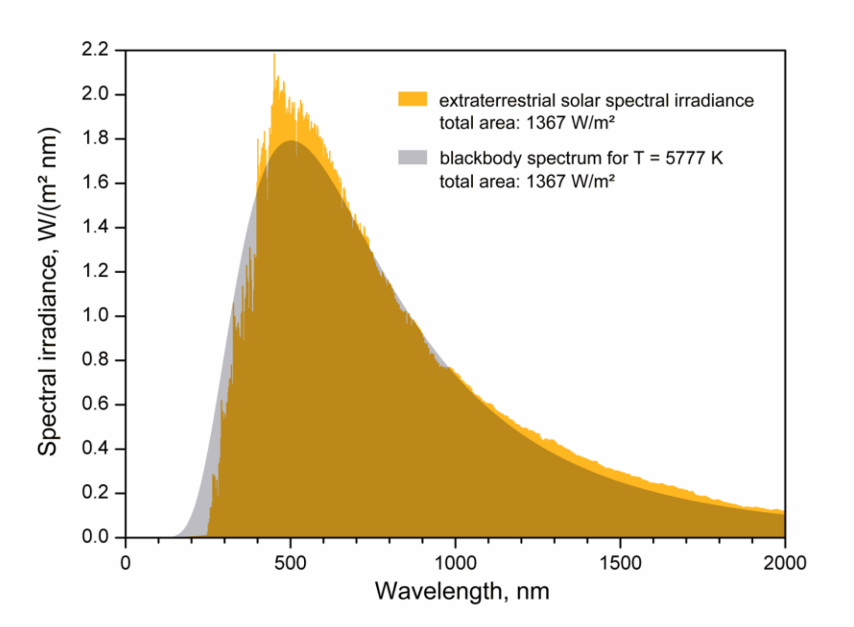
Planck and Maxwell

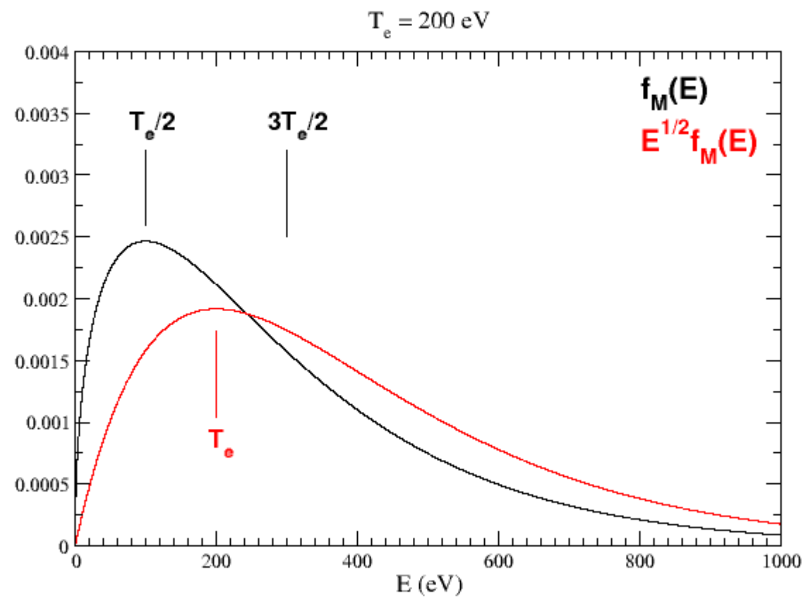
- Planck distribution

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



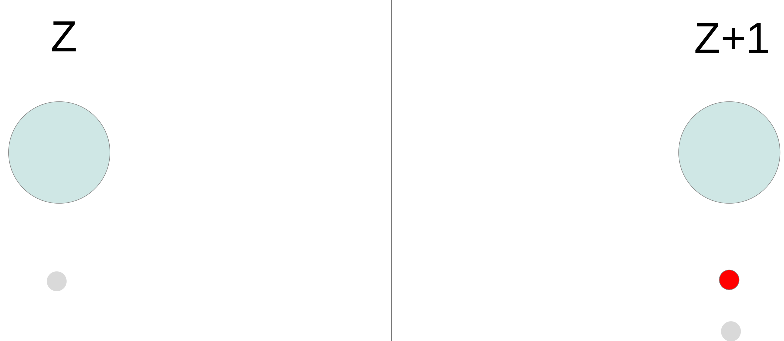
- Maxwell distribution

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



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**

- Griem's criterion for Boltzmann: *collisional rates > 10*radiative rates*

$$n_e[cm^{-3}] > 1.4 \times 10^{14}(\Delta E_{01}[eV])^3 (T_e[eV])^{1/2} \propto Z^7$$

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

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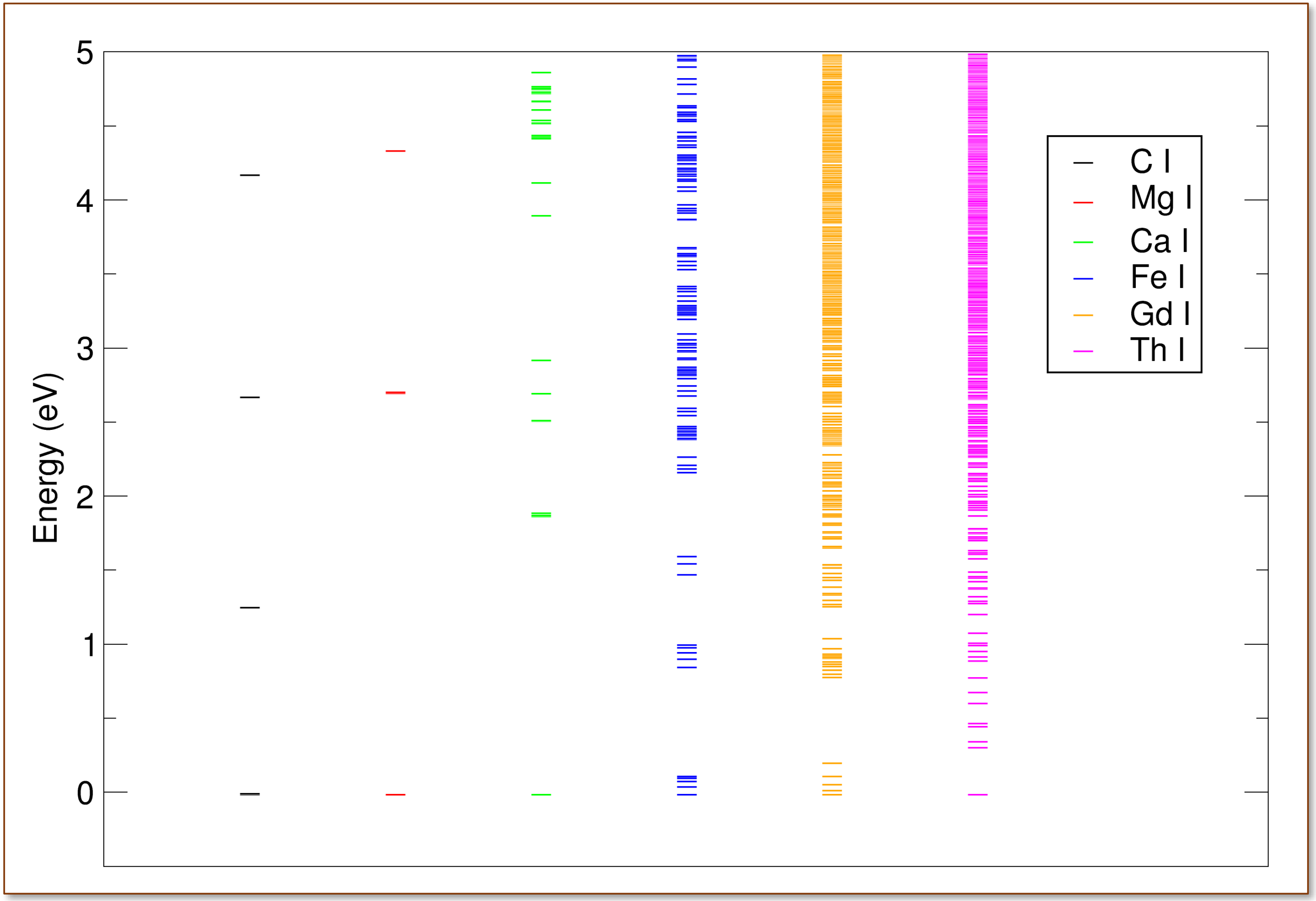
NIST ASD energy levels



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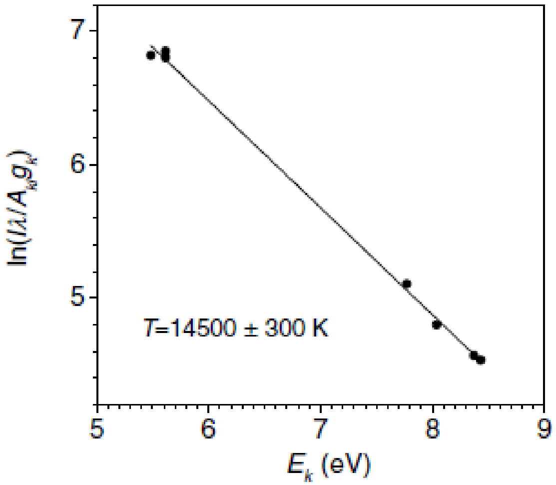
LTE Line Intensities

- ***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)

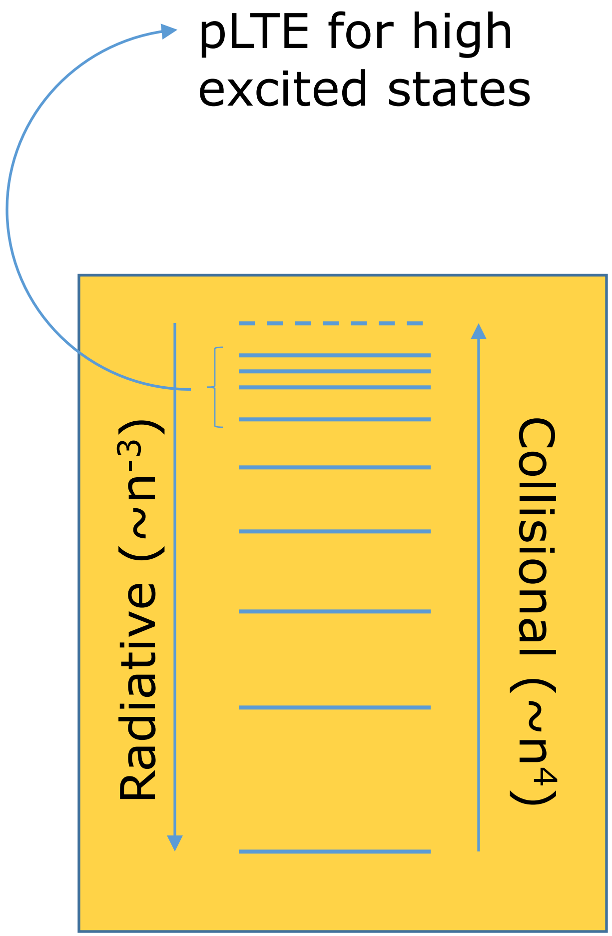
Saha-LTE conclusions

- Collisions >> radiative processes
  - Saha distribution between ions
  - Boltzmann distribution within ions
- Since collisions decrease with Z and radiative processes increase with Z, 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!!!

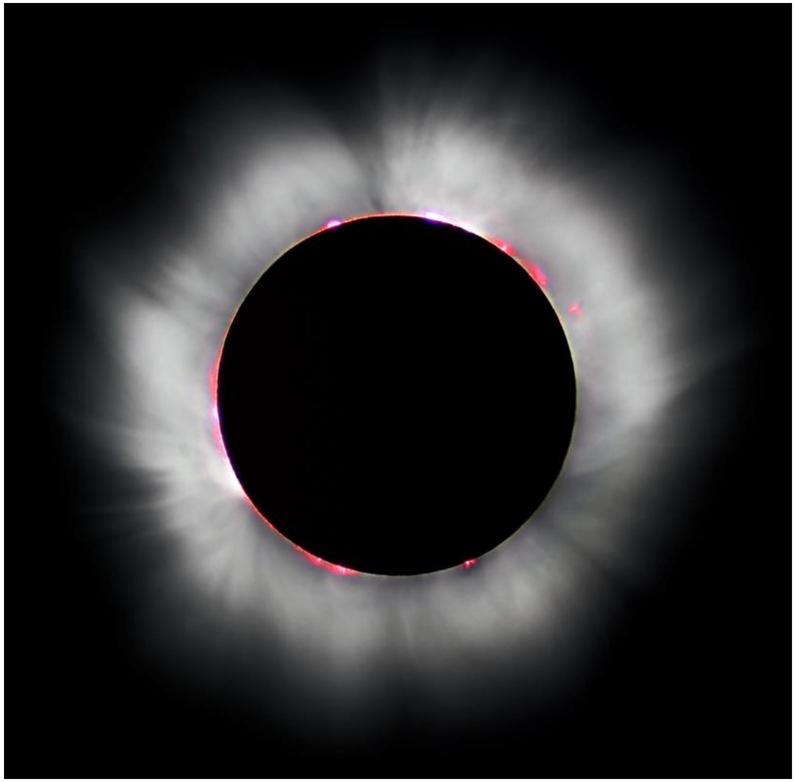
Deviations from LTE

- 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!



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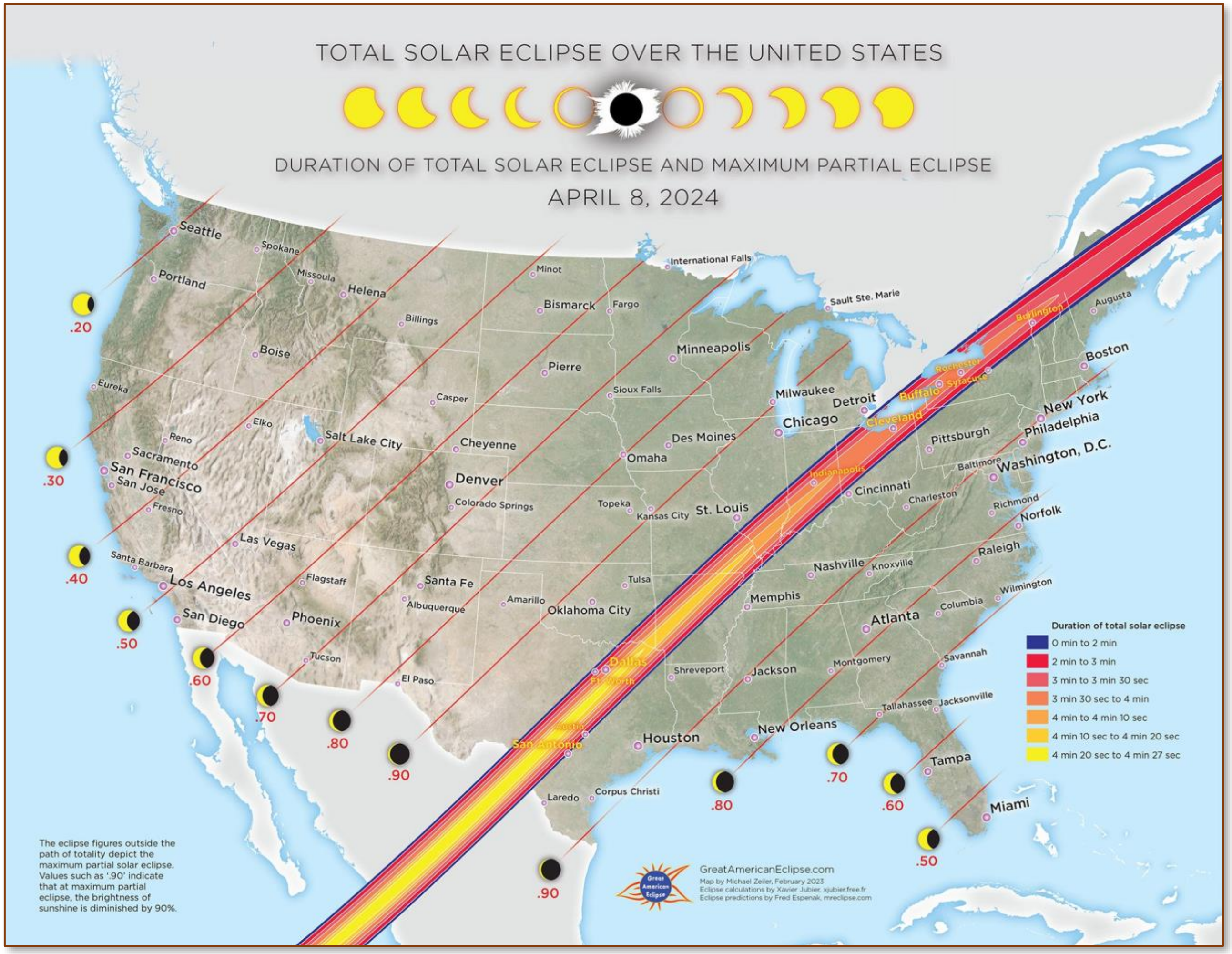
2nd Great American Eclipse: Apr 8



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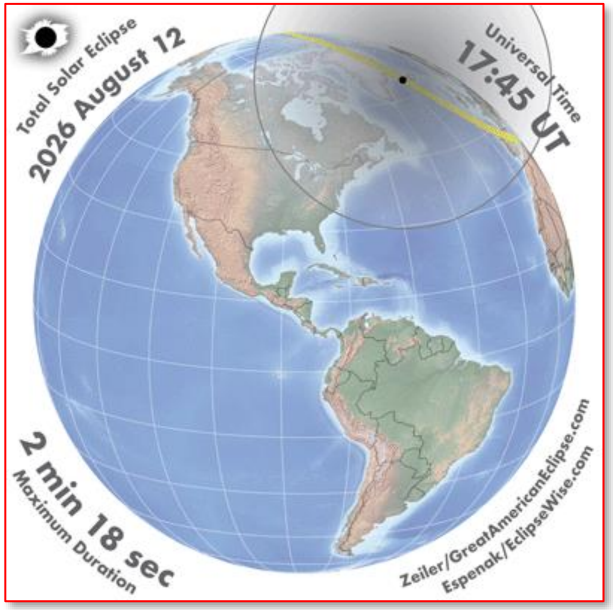

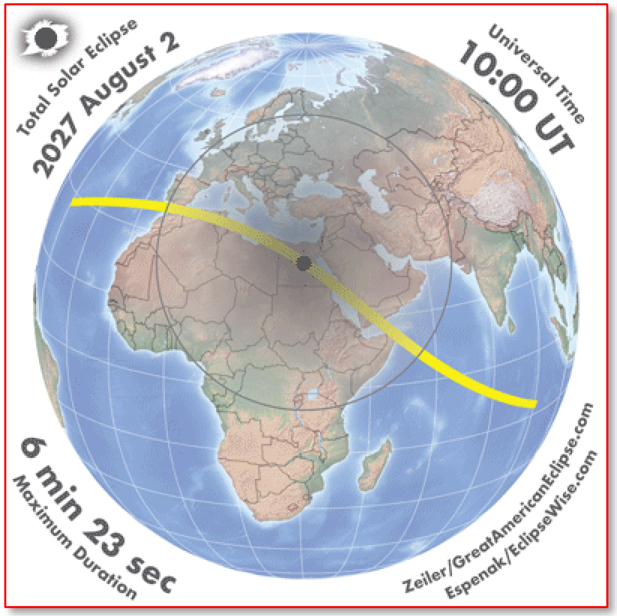

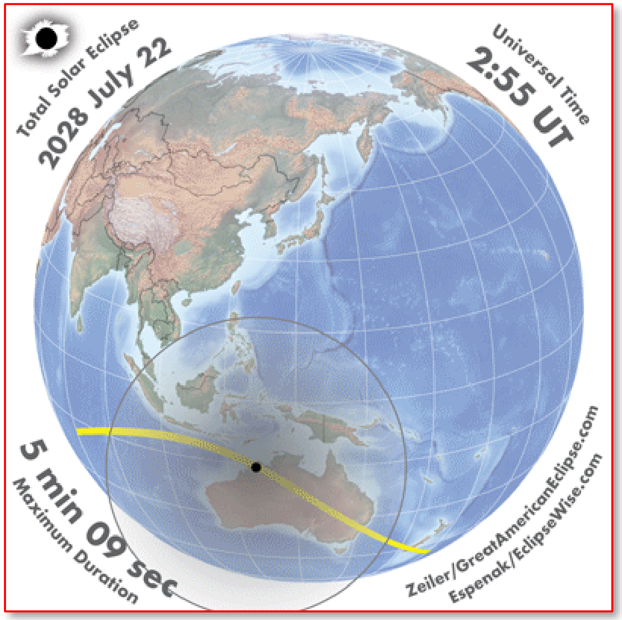

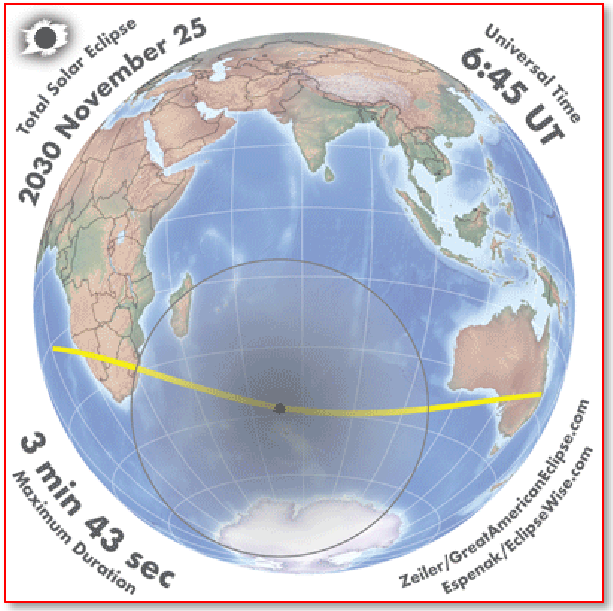

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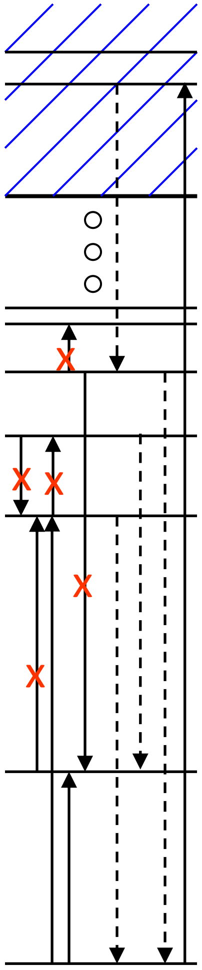
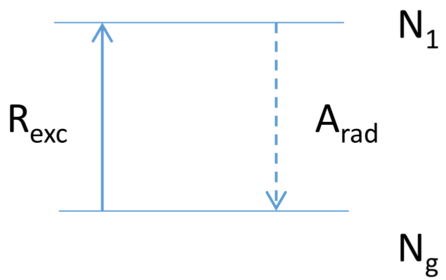
Coronal model

- 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?..



Line Intensities under CE



Balance equation:

small populations!

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

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

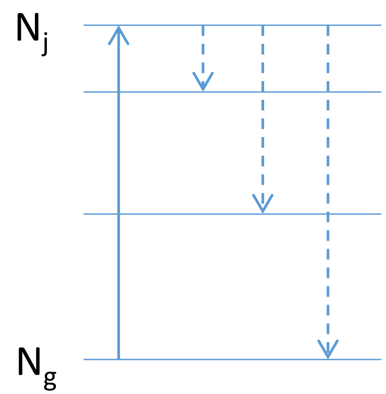
$$I = N_1 A_{rad} E = N_g R_{exc} E$$

Line intensity does NOT depend on A_{rad}!

$I \propto n_e$

Populations are small!!!

If more than one radiative transition:



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

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

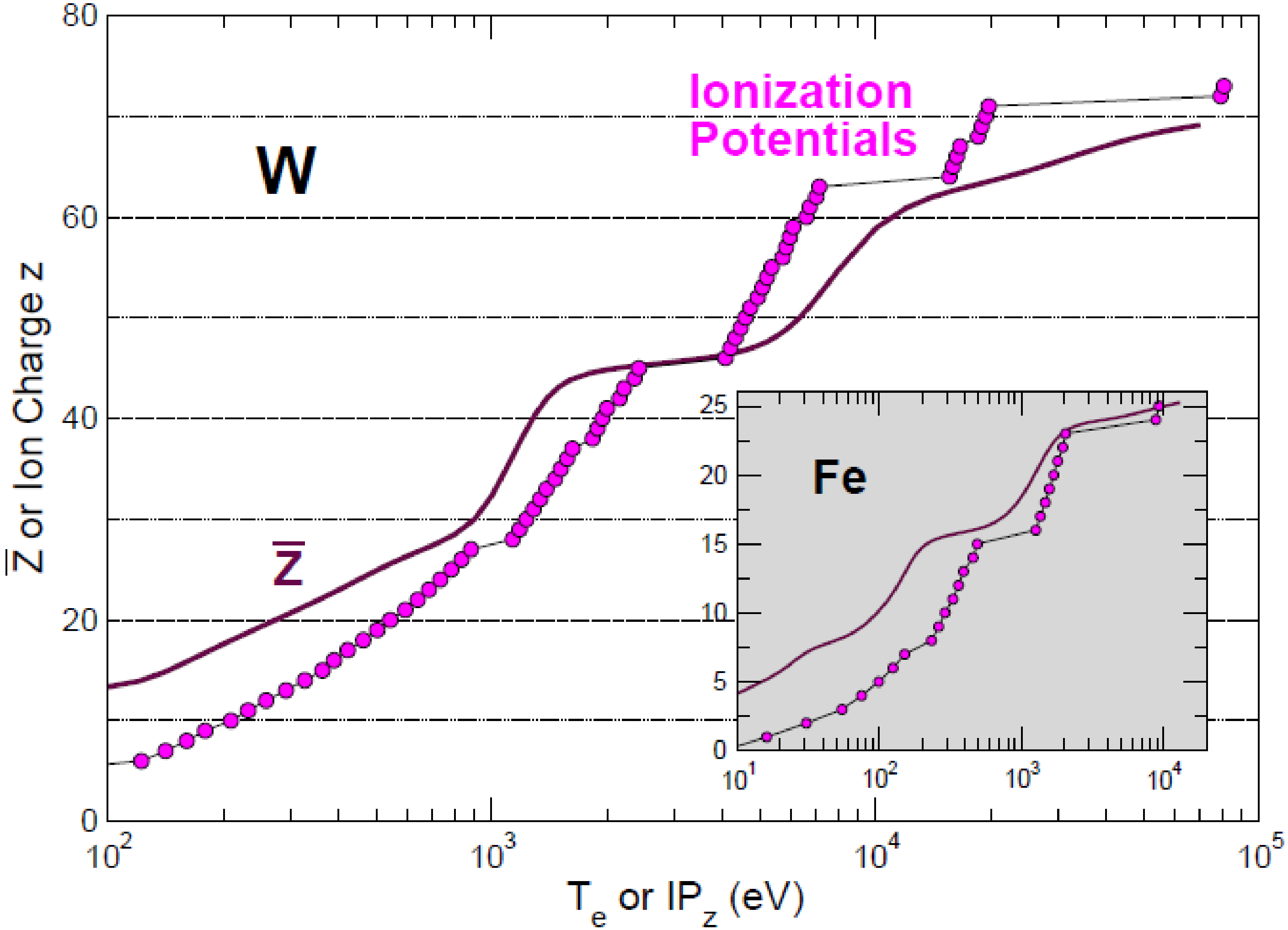
$$I_{ij} = N_j E_{ij} A_{ij}$$

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

Cascades may be important

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

Most Abundant Ions: high Z



Ionization decreases faster with Z than recombination: recombination becomes relatively stronger

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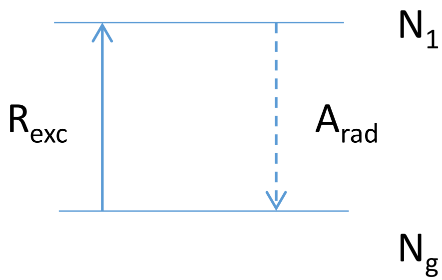
Time-Dependent Corona



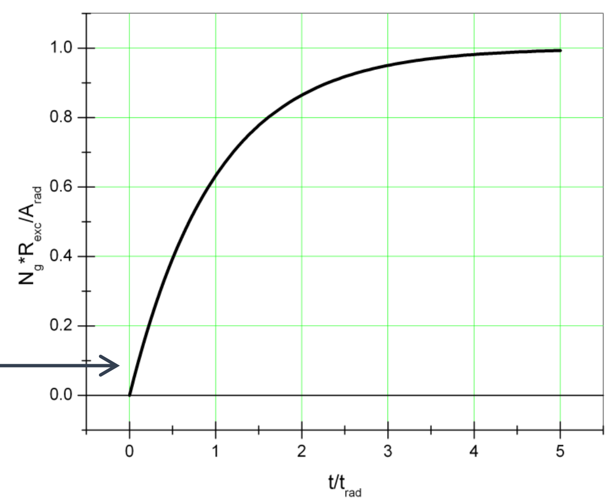
Initial condition: **$N_1(t=0) = 0$**

$$\frac{dN_1(t)}{dt} = N_g R_{exc} - N_1(t) A_{rad}$$

Solution: $$N_1(t) = \frac{N_g R_{exc}}{A_{rad}}\left(1 - e^{-A_{rad} t}\right)$$

Linear regime:

$N_1(t) \approx N_g R_{exc} t$

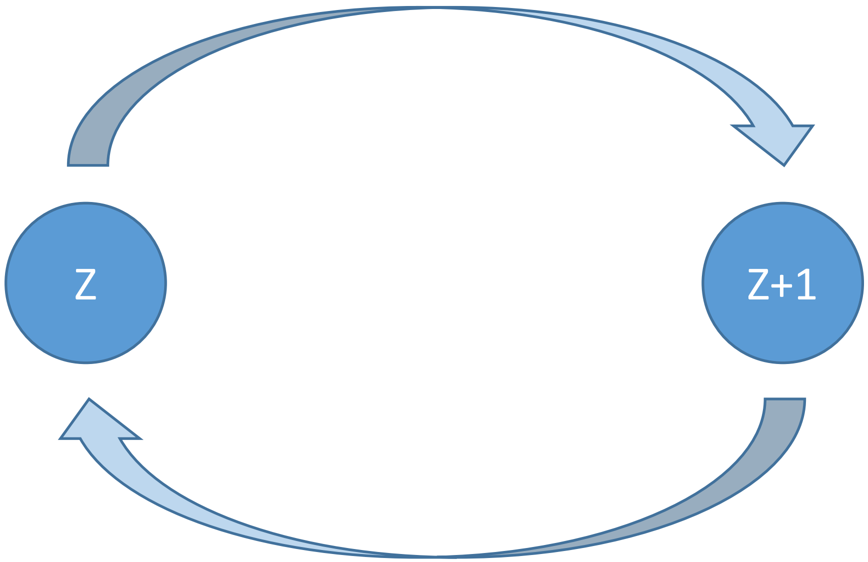


Characteristic time depends only on A_{rad}:

$$t_{eq} \approx t_{rad} = \frac{1}{A_{rad}}$$

Ionization Balance in CE

Electron-impact ionization: $\propto n_e$



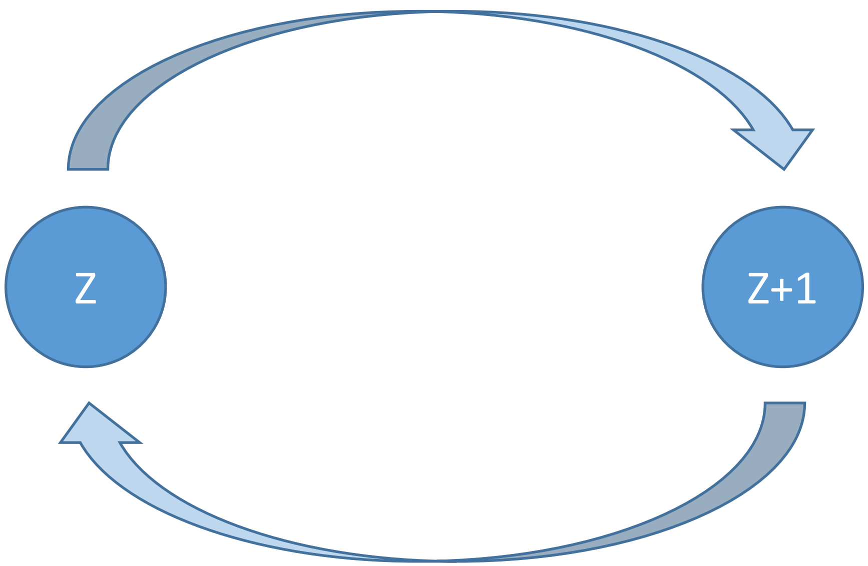
Photorecombination and DR: $\propto n_e$

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

Independent of n_e!

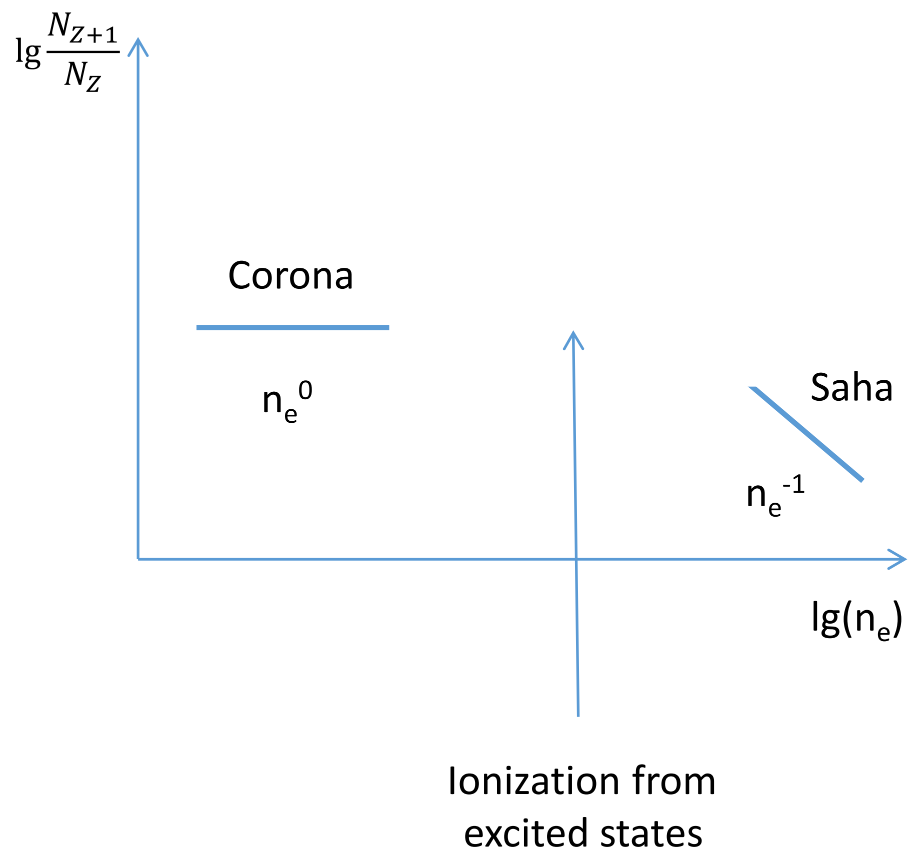
Ionization Balance in a General Case

Electron-impact ionization: $\propto n_e$

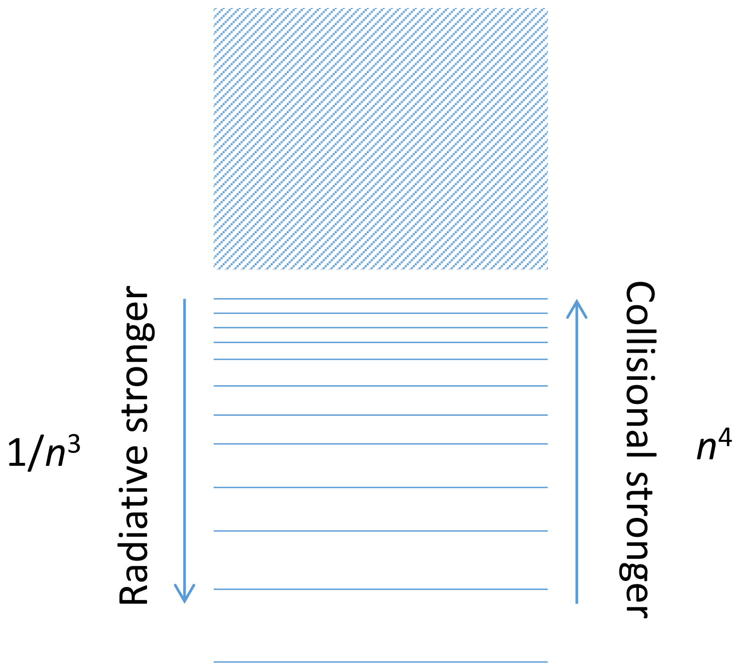


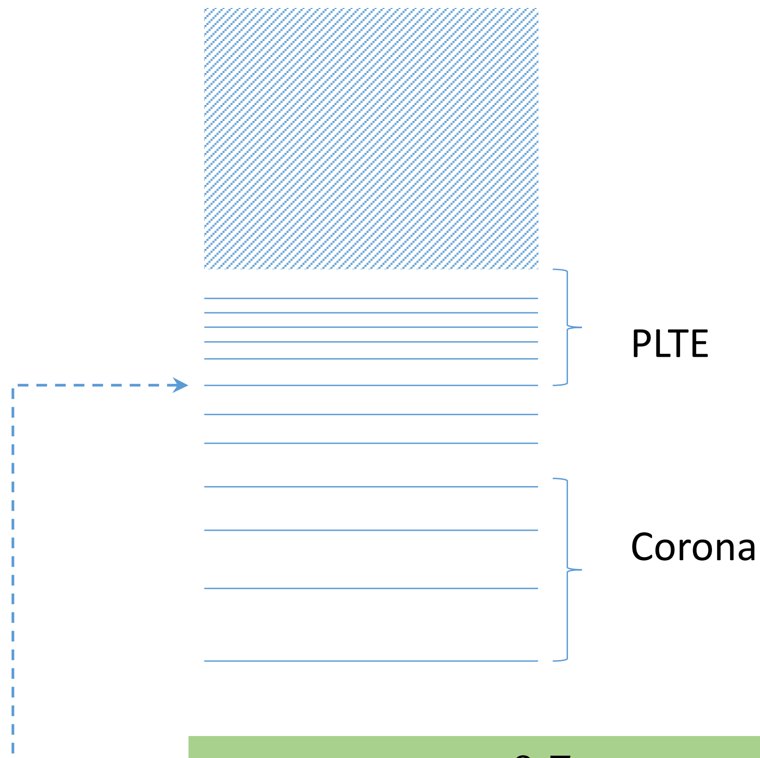
Photorecombination and DR: $\propto n_e$

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



From Corona to PLTE

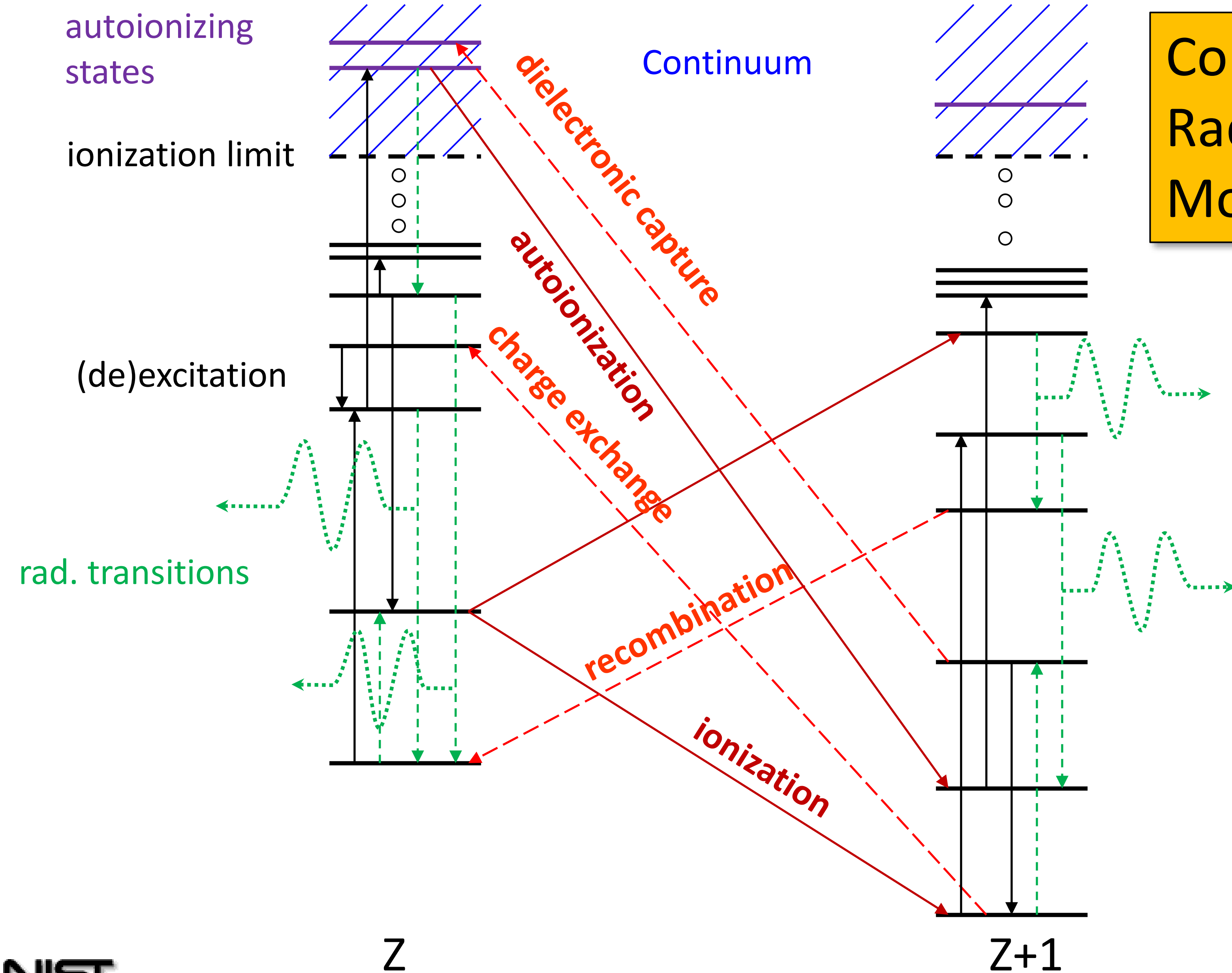




Griem limit:

$$n \sim 140 \cdot \frac{Z^{0.7}}{N_e^{2/17}} T_e^{1/17}$$

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)

$$\frac{dN_{Zi}}{dt} = \sum_{j<i} N_{Z,j}\left(R_{Z,ji}^{e-exc} + R_{Z,ji}^{h-exc} + B_{Z,ji}^{p-exc}\right)$$

$$+ \sum_{j>i} N_{Z,j}\left(R_{Z,ji}^{e-dexc} + R_{Z,ji}^{h-dexc} + A_{Z,ji}^{sp-rad} + B_{Z,ji}^{st-rad}\right)$$

$$+ \sum_{Z\prime>Z} \sum_{k\in Z\prime} N_{Z\prime,k}\left(\alpha_{Z\prime k,Zi}^{3b} + \alpha_{Z\prime k,Zi}^{rr} + \alpha_{Z\prime k,Zi}^{dc} + \alpha_{Z\prime k,Zi}^{cx}\right)$$

$$+ \sum_{Z\prime<Z} \sum_{k\in Z\prime} N_{Z\prime,k}\left(S_{Z\prime k,Zi}^{e-ion} + S_{Z\prime k,Zi}^{i-ion} + S_{Z\prime k,Zi}^{p-ion} + S_{Z\prime k,Zi}^{cx}\right)$$

$$-N_{Z,i} \times$$

$$(\sum_{j>i}\left(R_{Z,ij}^{e-exc} + R_{Z,ij}^{h-exc} + B_{Z,ij}^{p-exc}\right)$$

$$+ \sum_{j<i}\left(R_{Z,ji}^{e-dexc} + R_{Z,ji}^{h-dexc} + A_{Z,ji}^{sp-rad} + B_{Z,ji}^{st-rad}\right)$$

$$+ \sum_{Z\prime<Z} \sum_{k\in Z\prime}\left(\alpha_{Zi,Z\prime k}^{3b} + \alpha_{Zi,Z\prime k}^{rr} + \alpha_{Zi,Z\prime k}^{dc} + \alpha_{Zi,Z\prime k}^{cx}\right)$$

$$+ \sum_{Z\prime<Z} \sum_{k\in Z\prime}\left(S_{Zi,Z\prime k}^{e-ion} + S_{Zi,Z\prime k}^{i-ion} + S_{Zi,Z\prime k}^{p-ion} + S_{Zi,Z\prime k}^{cx}\right))$$

$$+S_i$$

CR model: features

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

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

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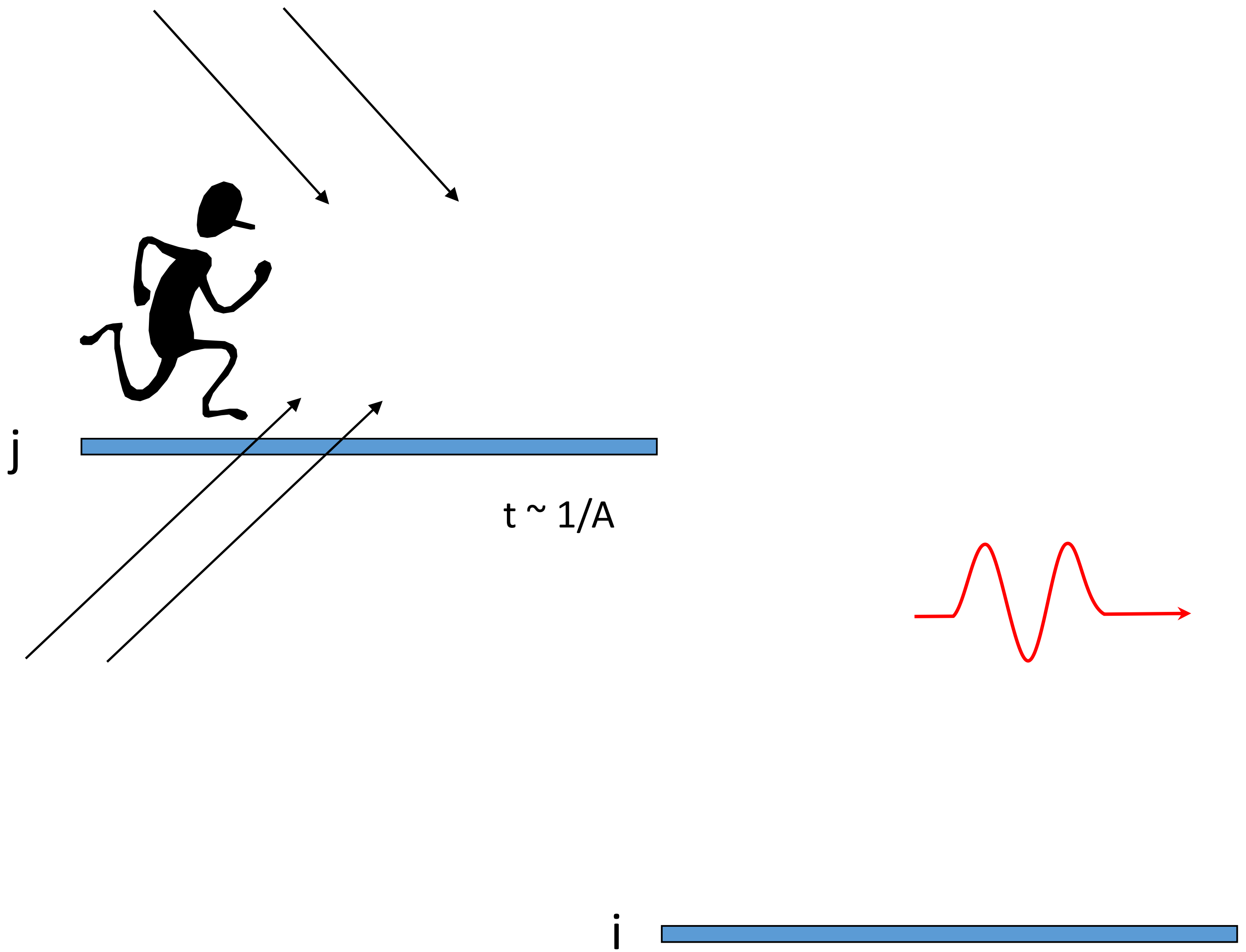
General principles for line intensity ratio diagnostics

- 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?



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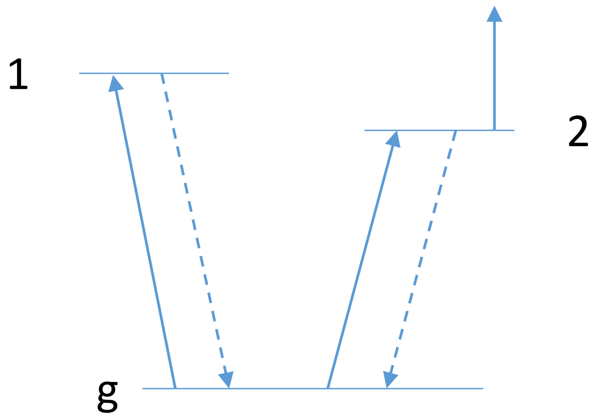
Let put it into a formula:

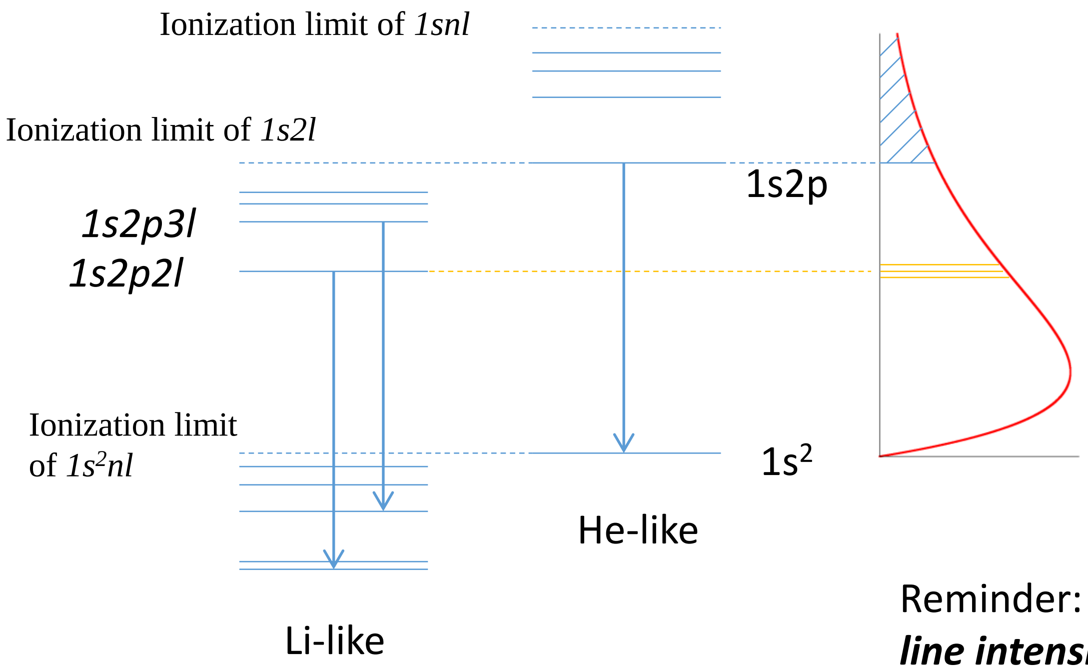


Strong transition

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

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

Temperature diagnostics with DS



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

DC rate for *1s2l2l'*~ $\dfrac{e^{-\frac{E_s}{T}}}{T^{3/2}}$

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!

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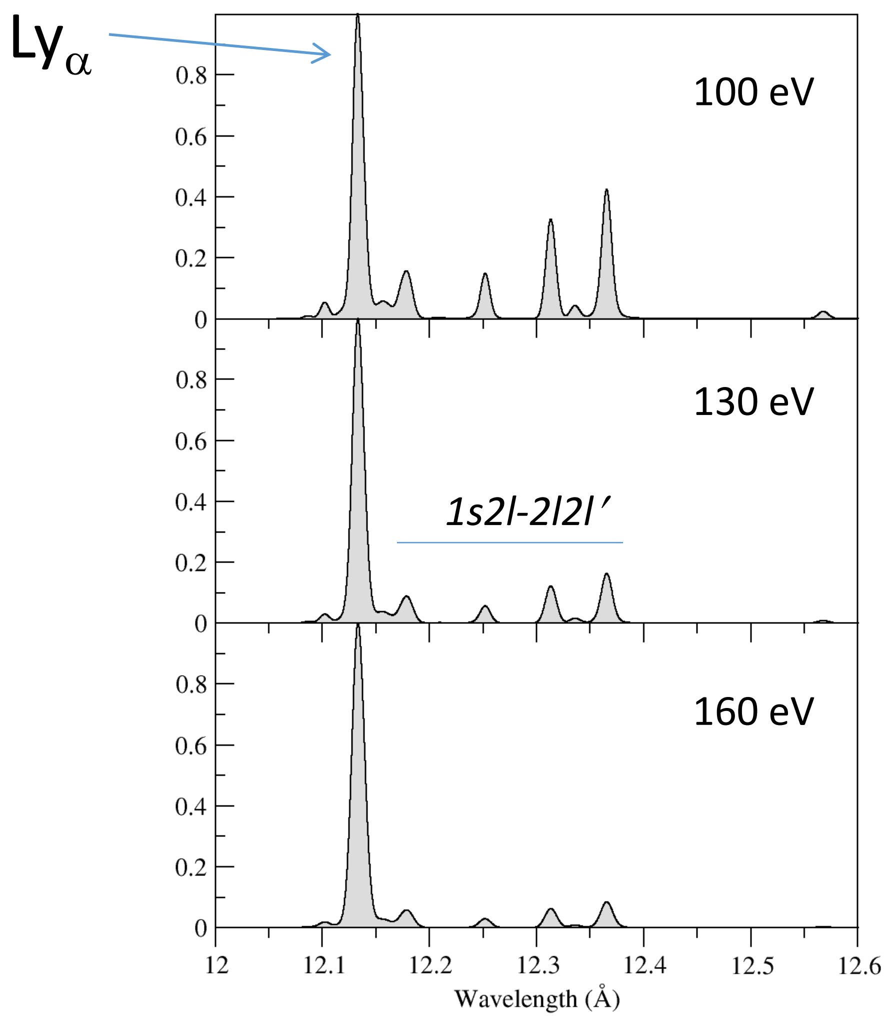
Temperature dependence: Ly_α satellites



H-like Ne X

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

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

1snl-2l′nl, n=2,3,4,…

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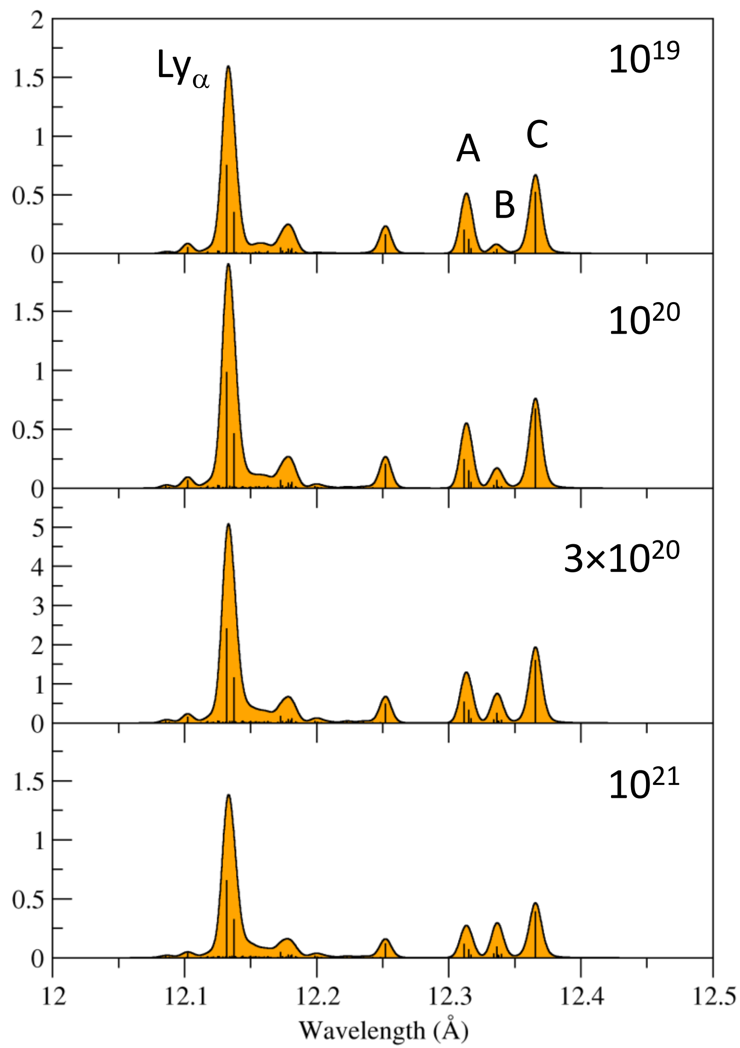
Density diagnostics with DS

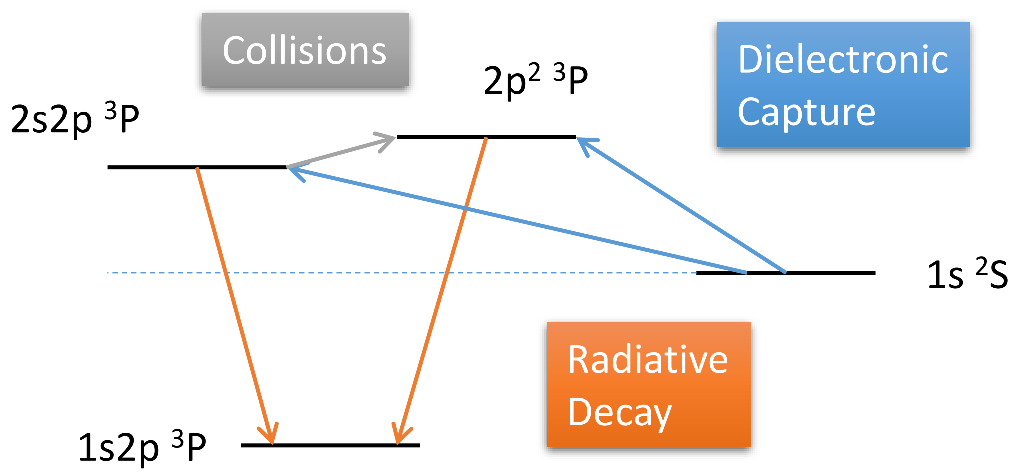


Ne X Ly$_\alpha$ and satellites *1snl-2pnl*

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)



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