Line Intensities, Collisional-Radiative Modeling…and everything else

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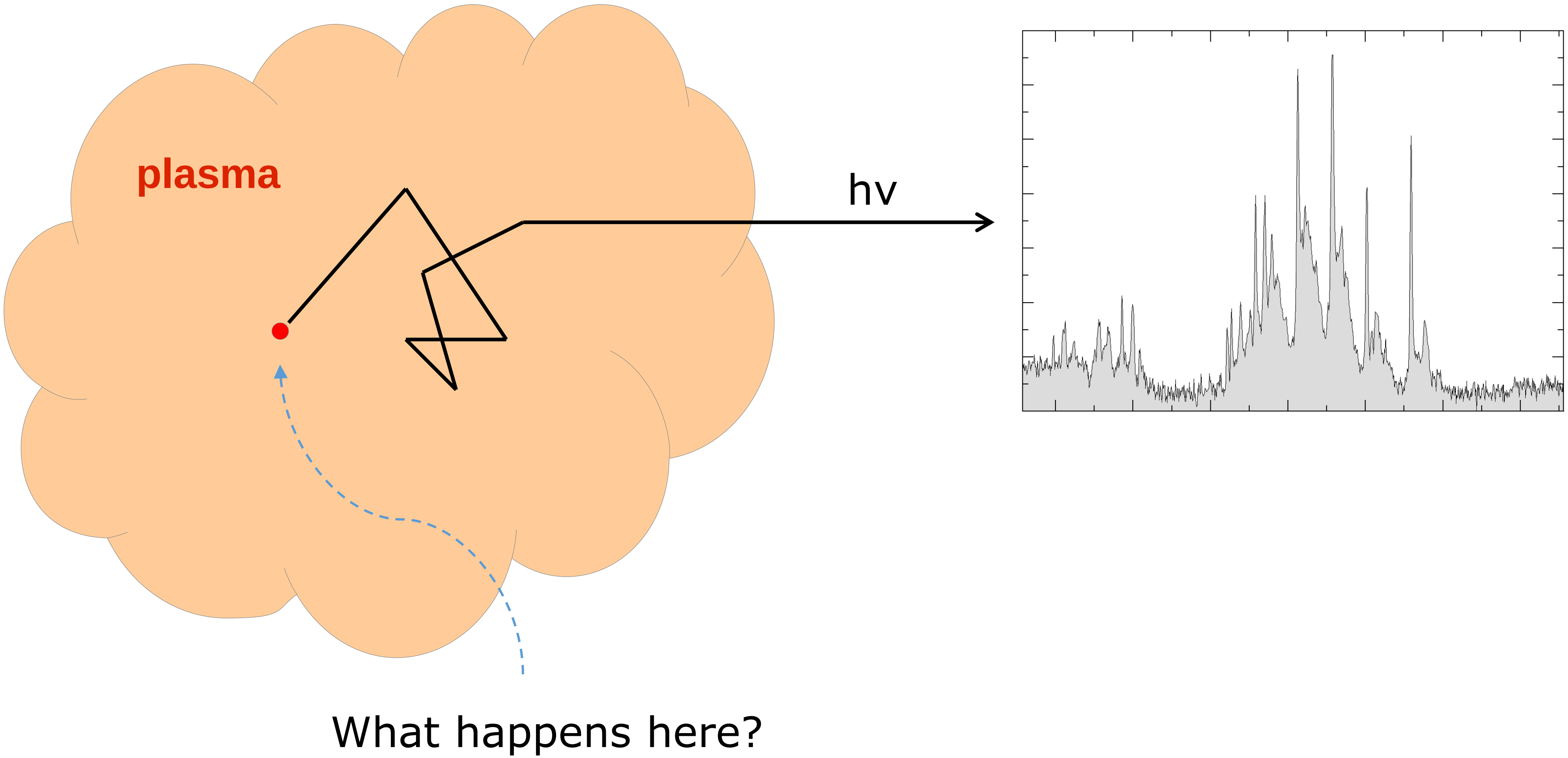
Where does the story begin?..



Spectral Line Intensity (optically thin)

Upper state density (cm^{-3})

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

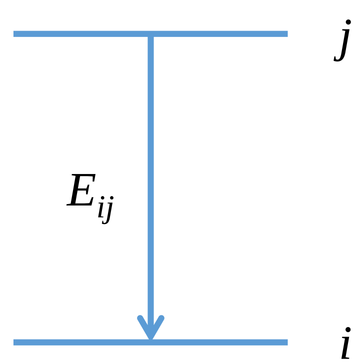
strongly depends on plasma conditions

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

(*almost*) purely atomic parameters

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

Photon energy (J)



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Rates

velocity [cm/s]

Collisional: $$R_{ij} = N_p \cdot \int \mathrm{v}\, \sigma_{ij}(\mathrm{v})\; f_p(\mathrm{v})\, d\mathrm{v}$$ [s^{-1}]

projectile density [cm^{-3}]

cross section [cm^2]

Radiative: 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
    - $A \sim n^{-3}$

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

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

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

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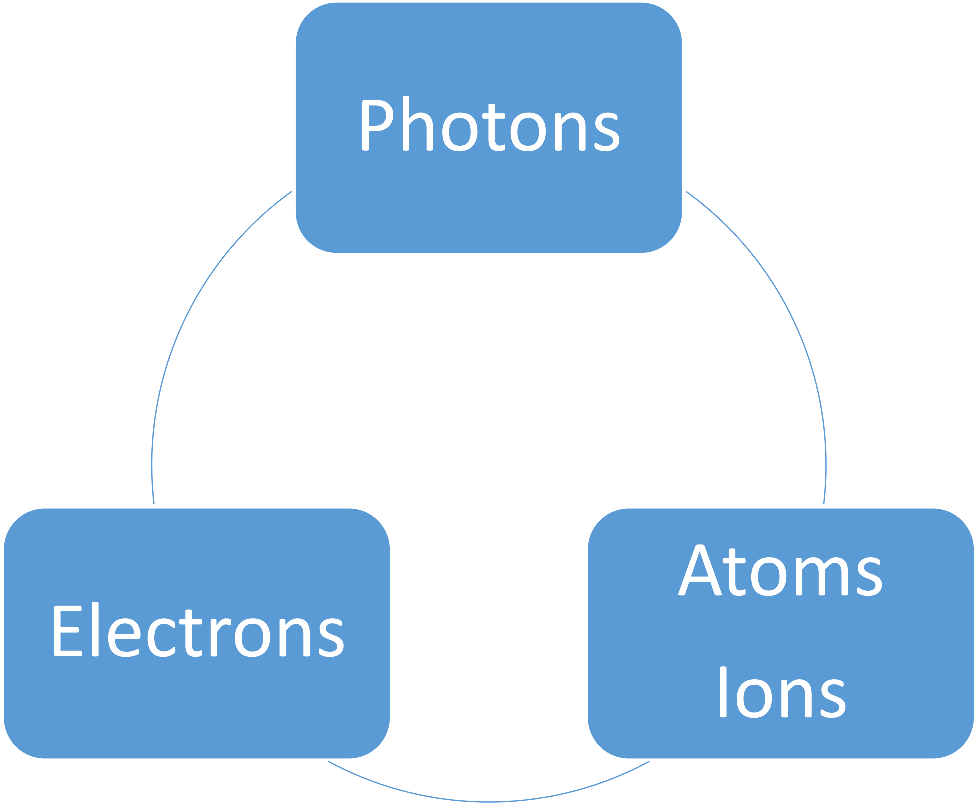
Thermodynamic equilibrium

- 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



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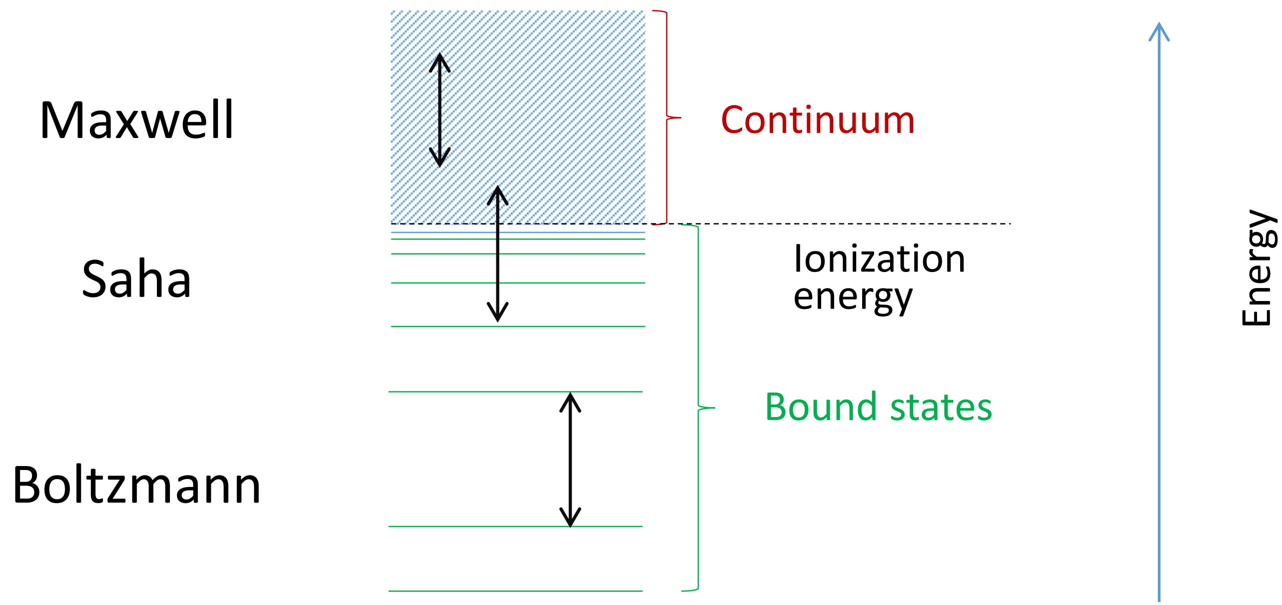
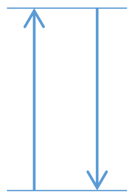
TE: distributions

- 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

TE: energy scheme



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



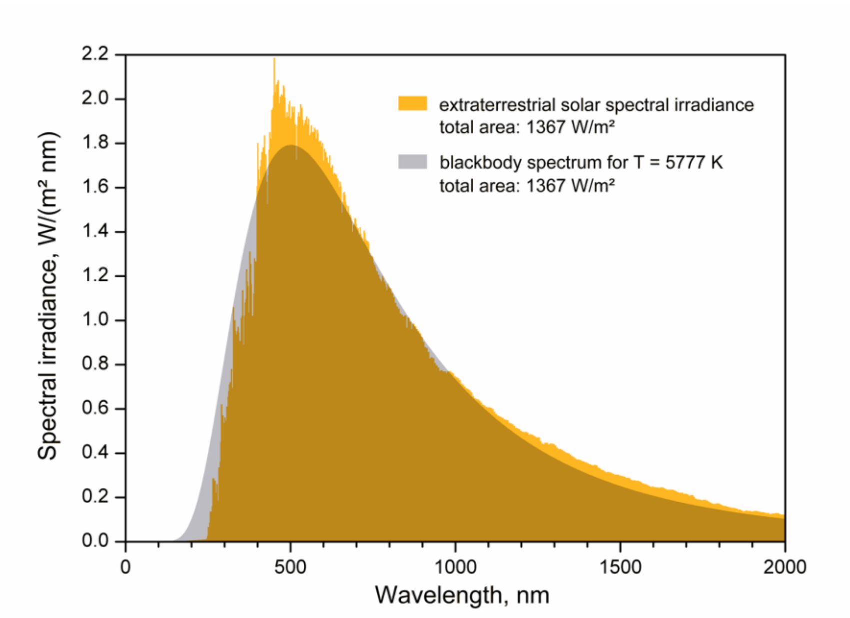
Planck and Maxwell

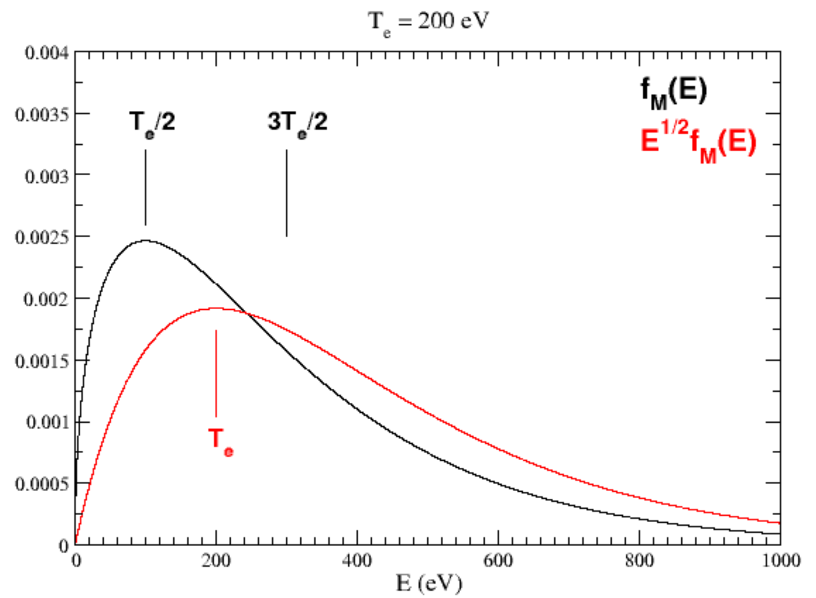
- Planck distribution

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

- Maxwell distribution

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





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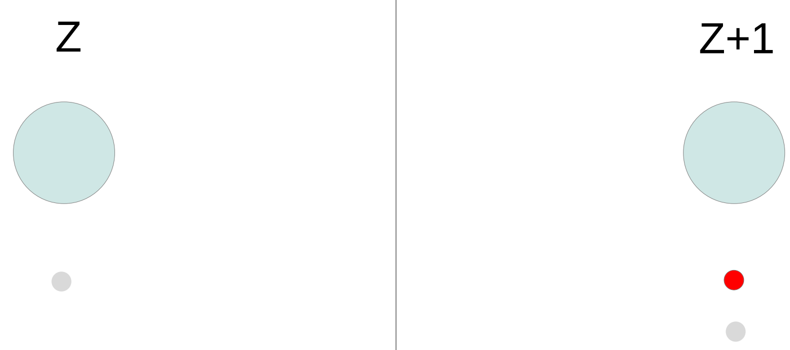
Saha Distribution

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*

$$N_e\left[cm^{-3}\right] > 1.4\times10^{14}\left(\Delta E_{01}\left[eV\right]\right)^3\left(T_e\left[eV\right]\right)^{1/2} \propto Z^7$$

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

- Saha criterion **for low T_e**:

$$N_e\left[cm^{-3}\right] > 1\times10^{14}\left(I_z\left[eV\right]\right)^{5/2}\left(T_e\left[eV\right]\right)^{1/2} \propto Z^6$$

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

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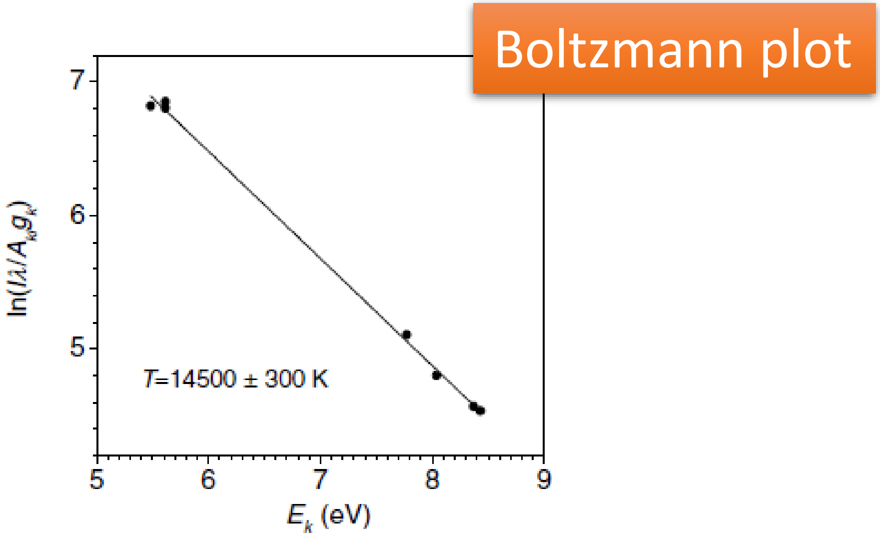
LTE Line Intensities

- ***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:

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

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



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

Saha-LTE conclusions

- Collisions >> radiative processes
  - Saha between ions
  - Boltzmann 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}

ASD: can calculate Saha/LTE spectra!!!

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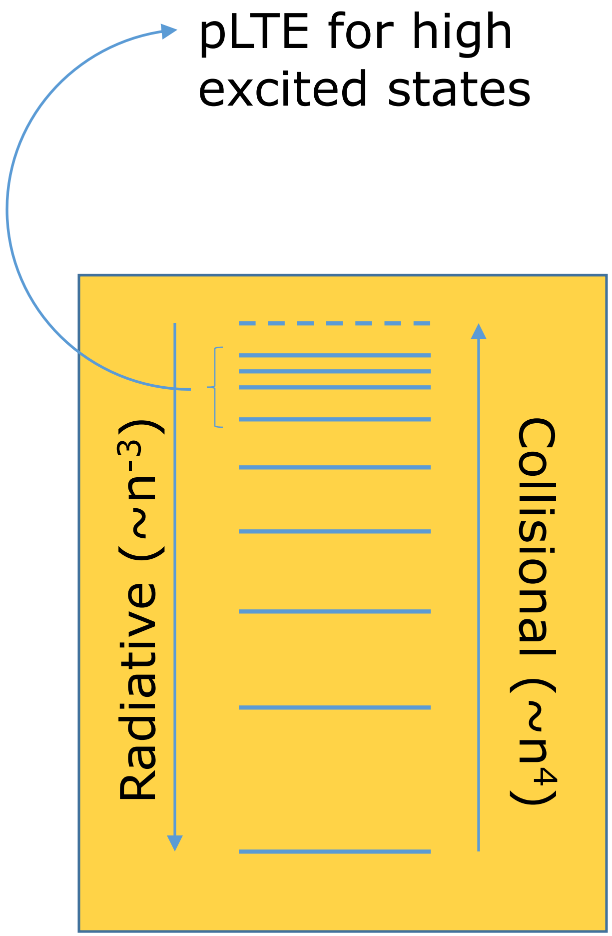
Deviations from LTE

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



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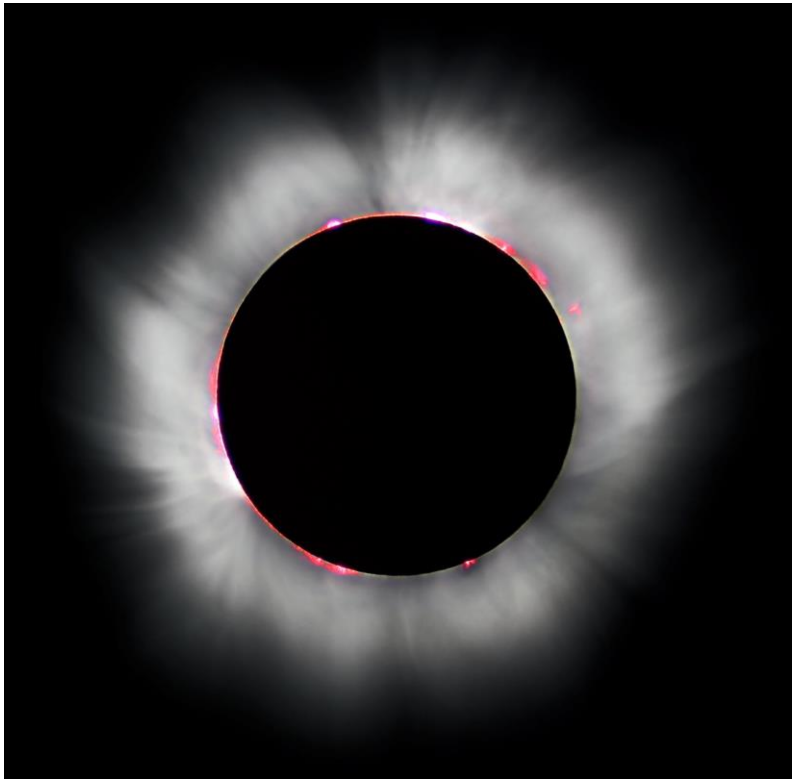
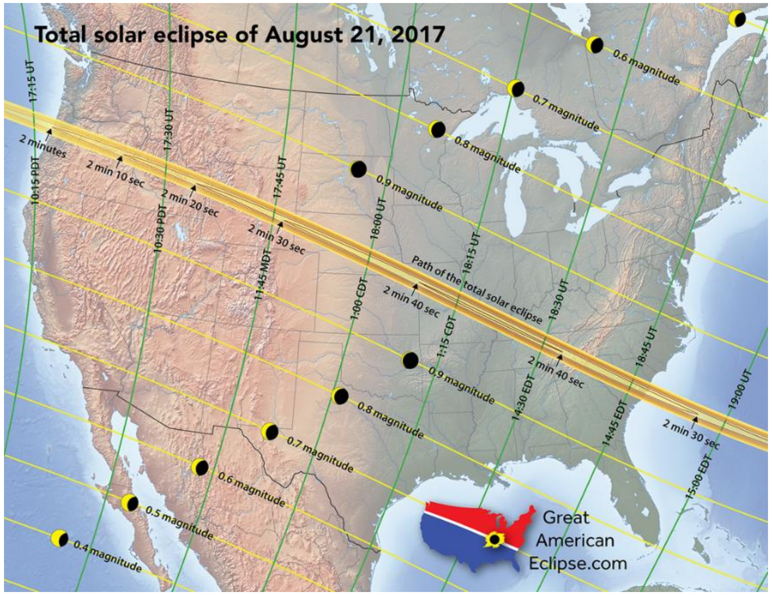
The other limiting case: Coronal Equilibrium

Low electron densities!



Next big: Aug 21, 2017



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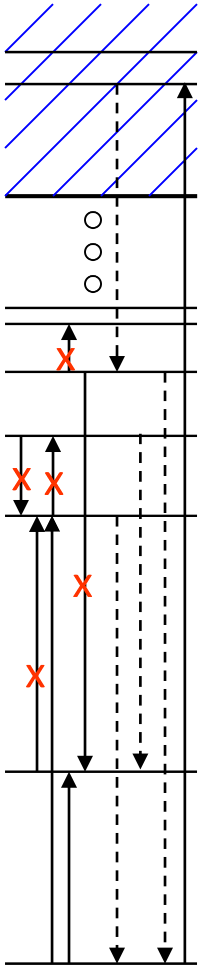
Coronal model

- 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?..



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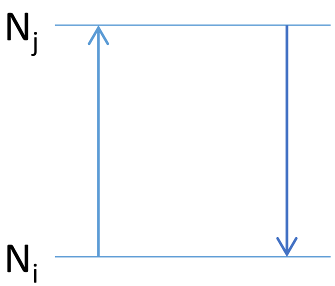
Excitation ↔ Deexcitation



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:

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

$$g_i \int_{\Delta E}^{\infty} \left(\frac{2E}{m}\right)^{1/2} \sigma_{ij}(E) E^{1/2} e^{-\frac{E}{T}} dE = g_j e^{-\frac{\Delta E}{T}} \int_0^{\infty} \left(\frac{2E'}{m}\right)^{1/2} \sigma_{ji}(E') E'^{1/2} e^{-\frac{E'}{T}} dE'$$

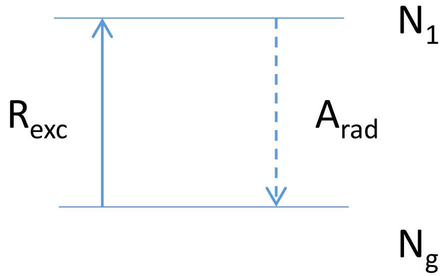
Only Maxwell is needed here!

Substitution: E ⇒ E+ΔE

$$g_i \int_0^{\infty} \left(E + \Delta E_{ij}\right) \sigma_{ij}(\varepsilon + \Delta E) e^{-\frac{E}{T}} dE = g_j \int_0^{\infty} E\, \sigma_{ji}(E) e^{-\frac{E}{T}} dE$$

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

Line Intensities under CE



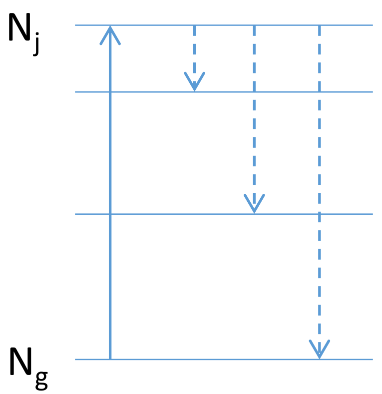
Balance equation:

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

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

small populations!

If more than one radiative transition:



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

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

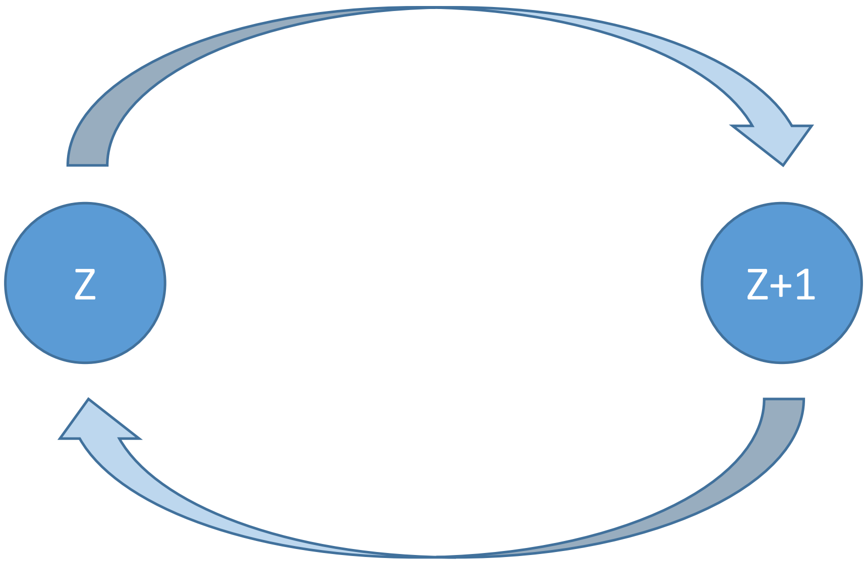
$$I_{ij} = N_j E_{ij} A_{ij} = N_g N_e \langle v\sigma_{jg} \rangle \frac{A_{ij}}{\sum_{k<j} A_{kj}}$$

Also cascades may be important

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

Ionization Balance in CE

Electron-impact ionization: $\propto N_e$



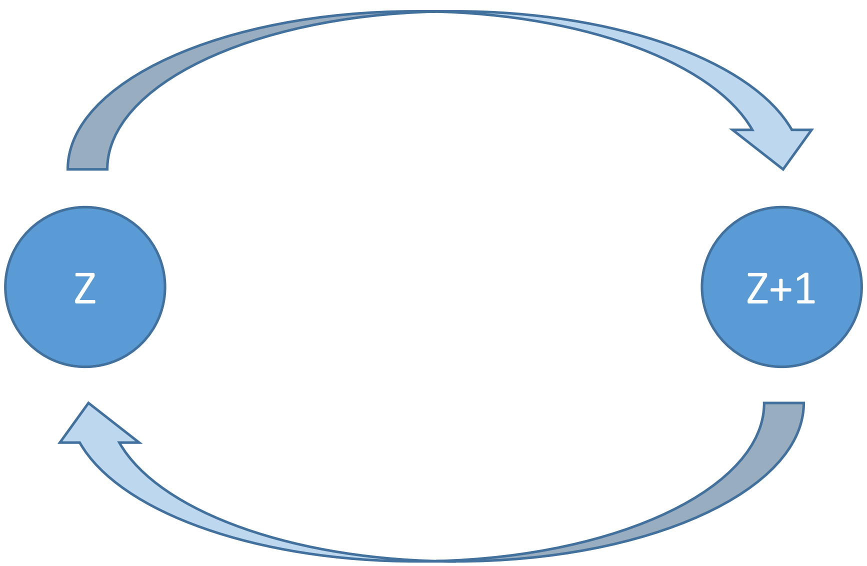
Photorecombination and DR: $\propto N_e$

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

Independent of N_e!

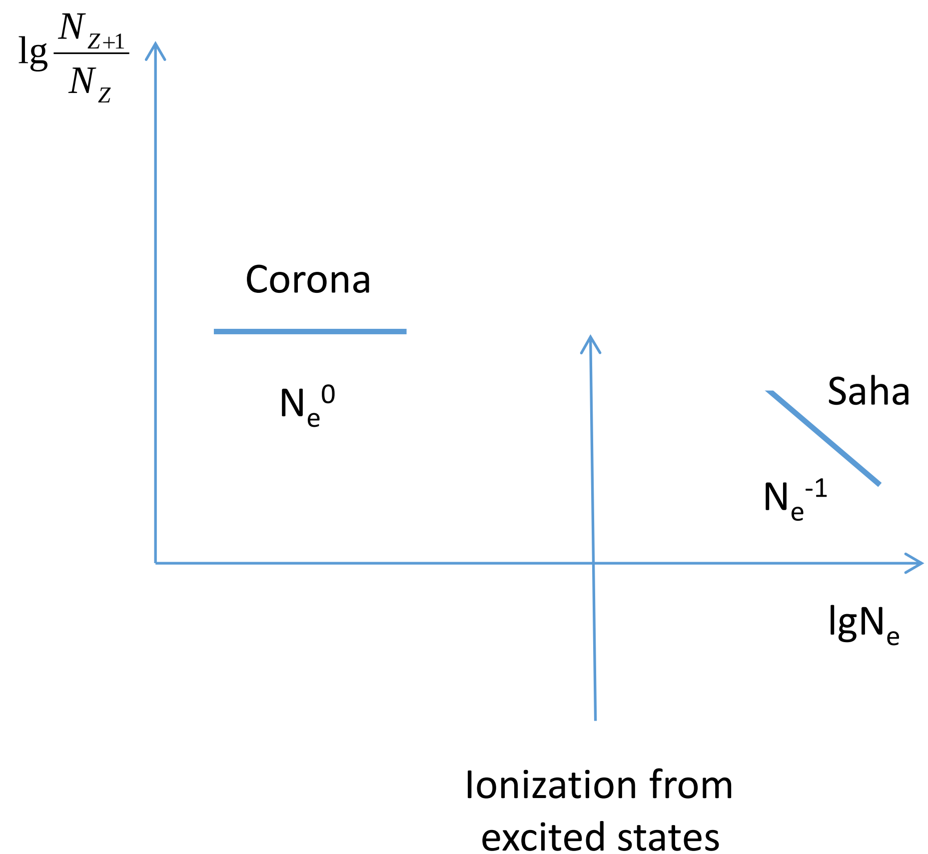
Ionization Balance in a General Case

Electron-impact ionization: $\propto N_e$

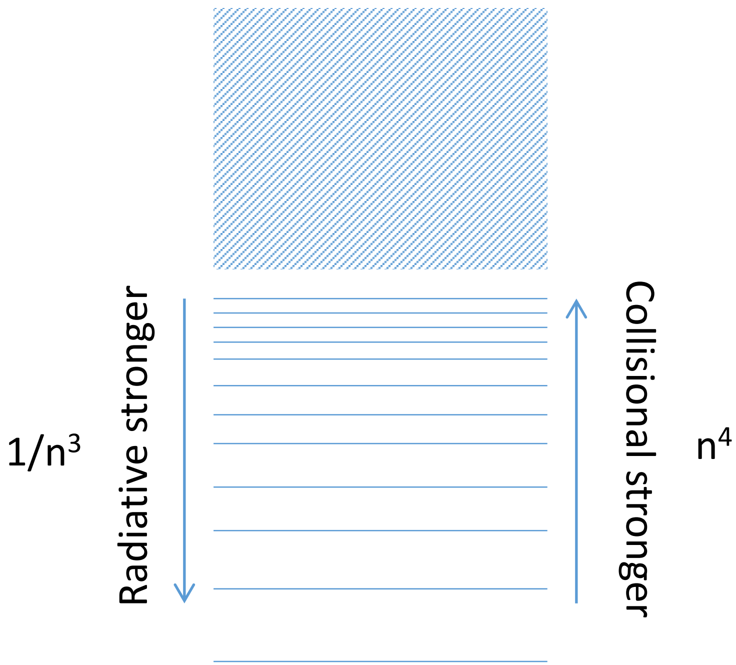


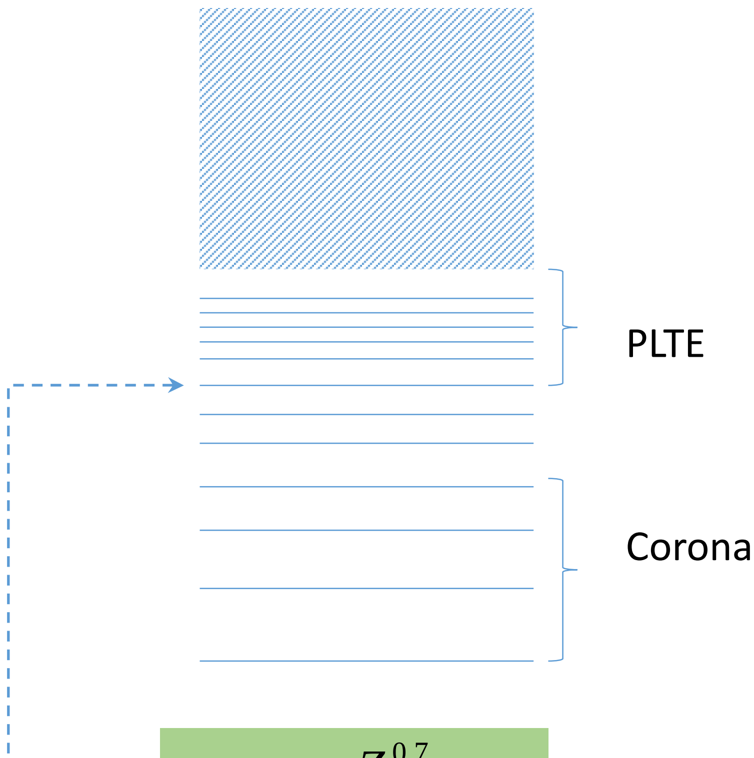
Photorecombination and DR: $\propto N_e$

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



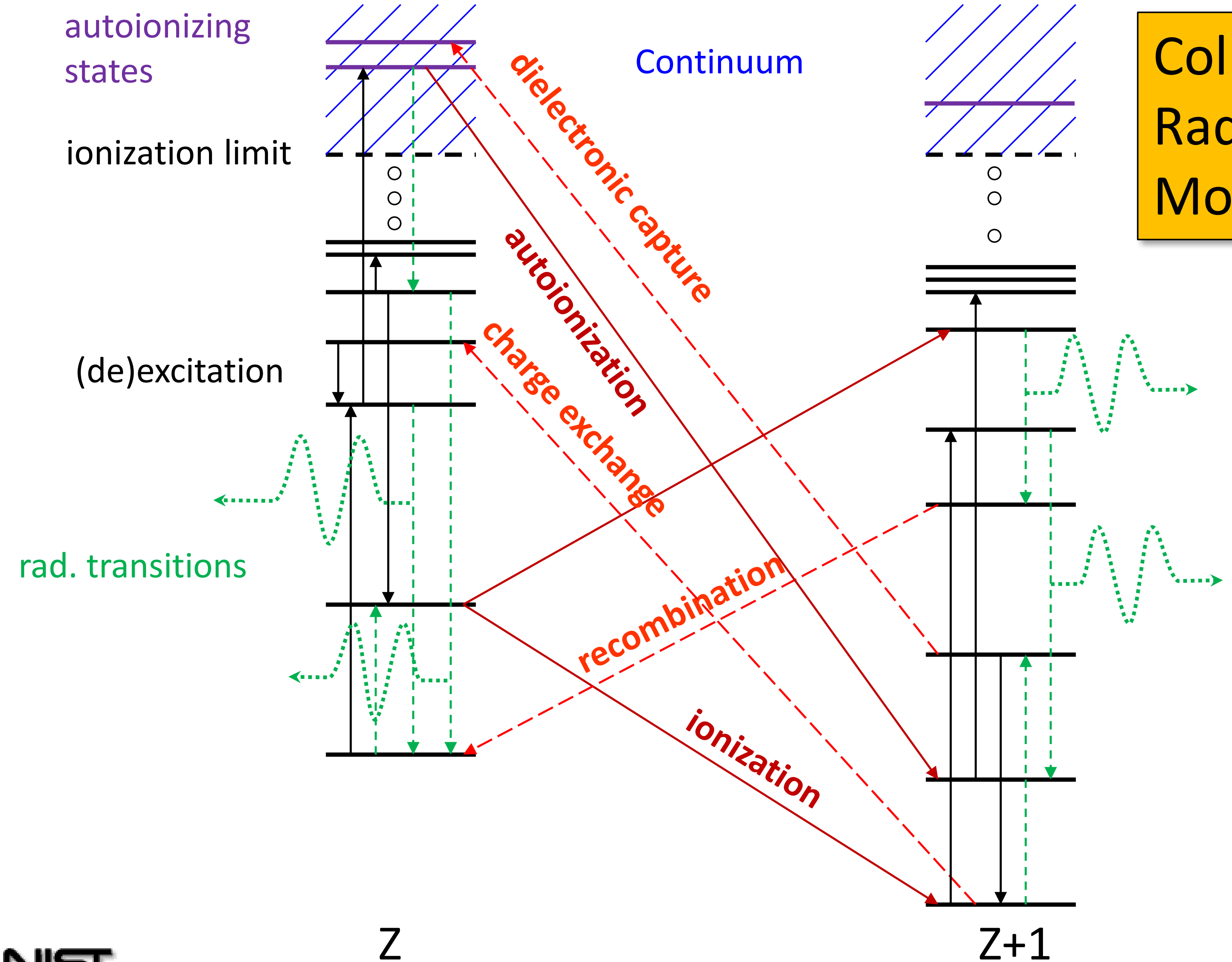
From Corona to PLTE





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

Collisional-Radiative Model



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Basic rate equation

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

Vector of atomic states populations

$$\frac{d\hat{N}(t)}{dt} = \hat{A}\left(t, \hat{N}(t), N_e, N_i, T_e, T_i \dots\right) \cdot \hat{N}(t) + \hat{S}(t)$$

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)

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

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

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

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

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

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

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

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

$$+ S_i$$

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 at low
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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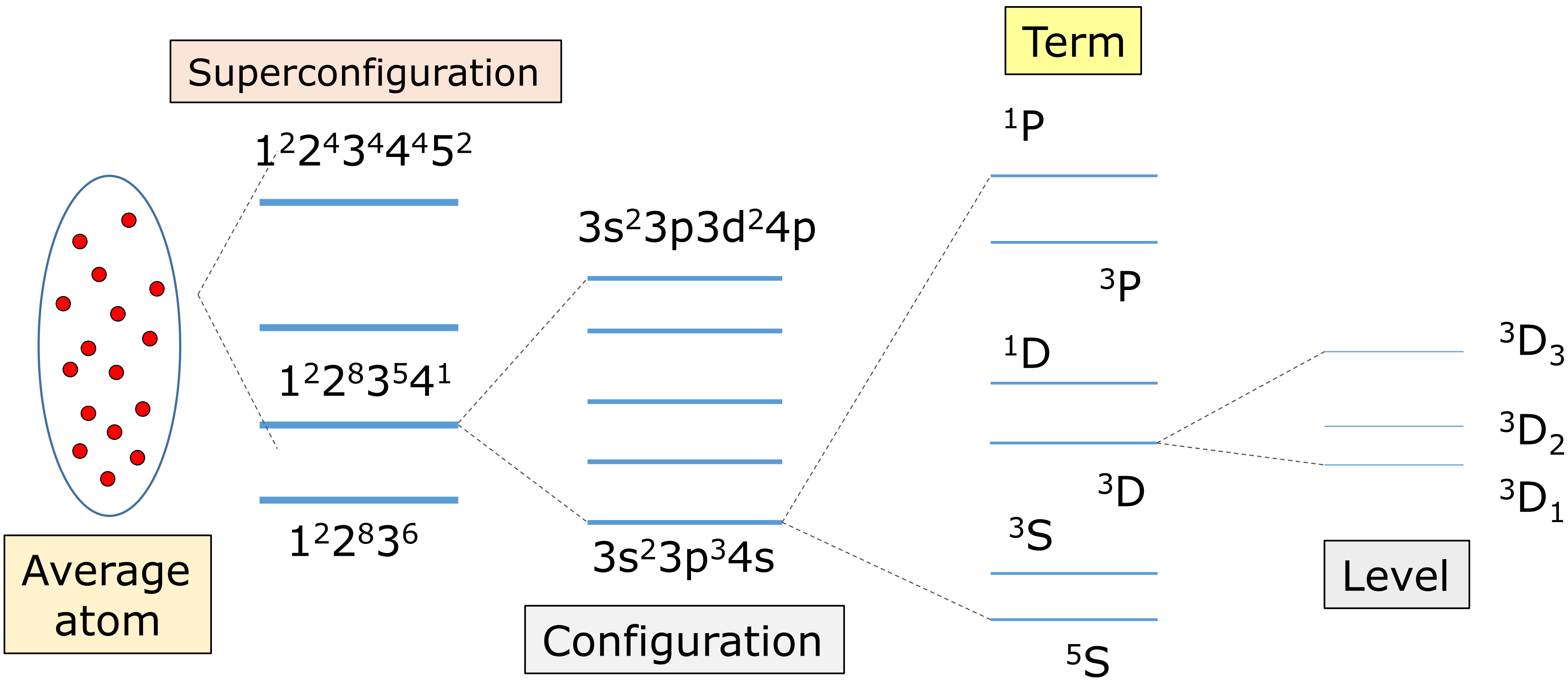
16-electron ion (S-like)



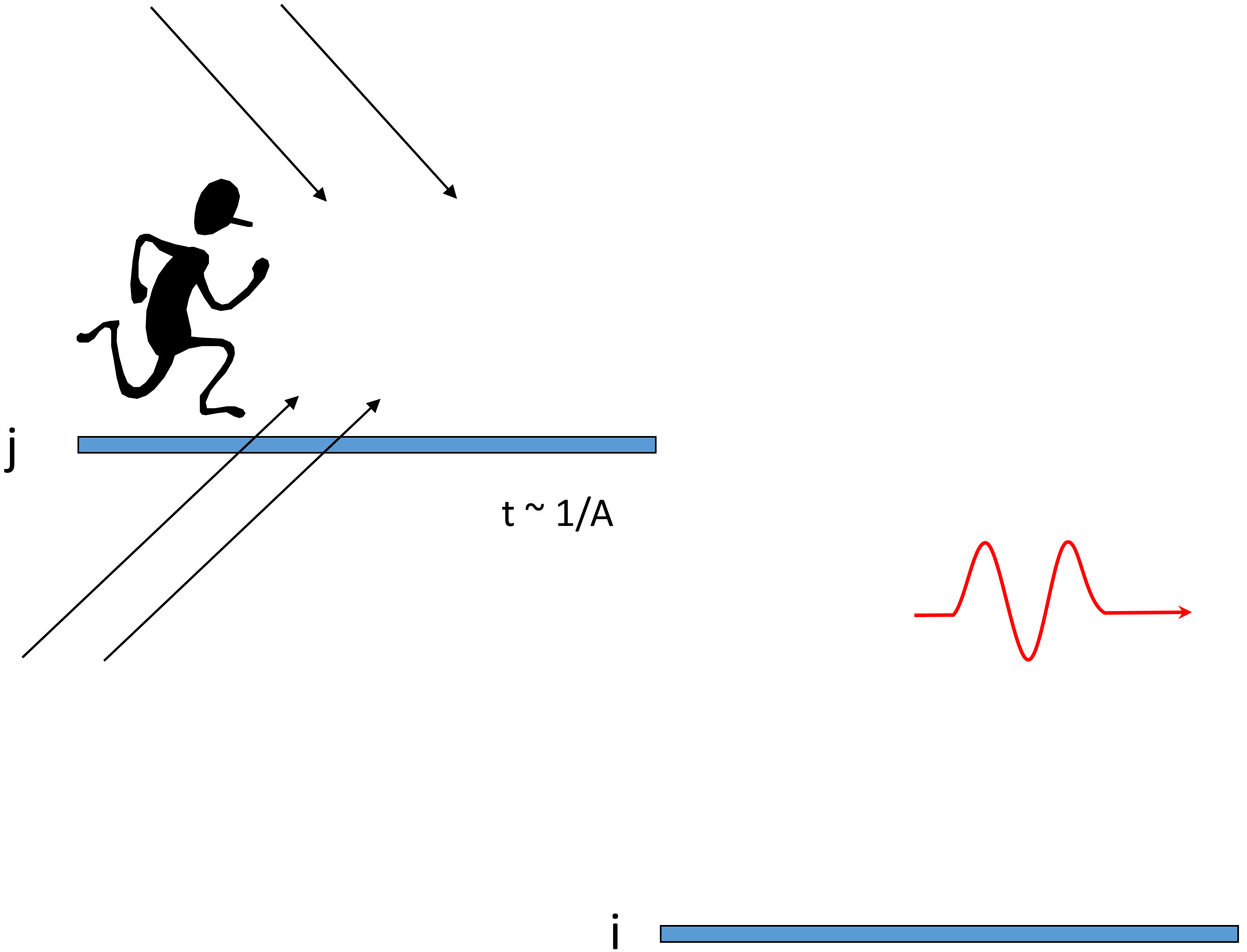
Even parabolic states for motional Stark effect!

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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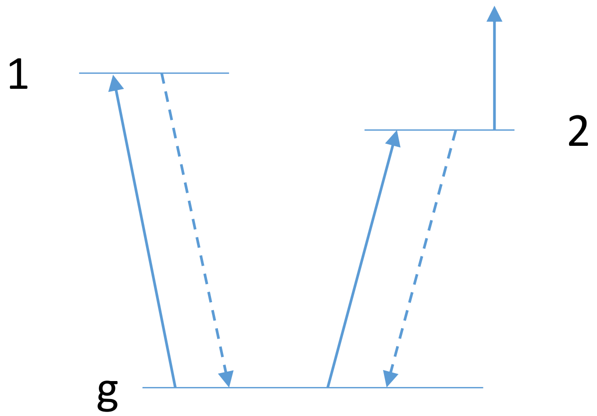
Let put him into a formula:

Strong transition

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

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



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

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

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

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

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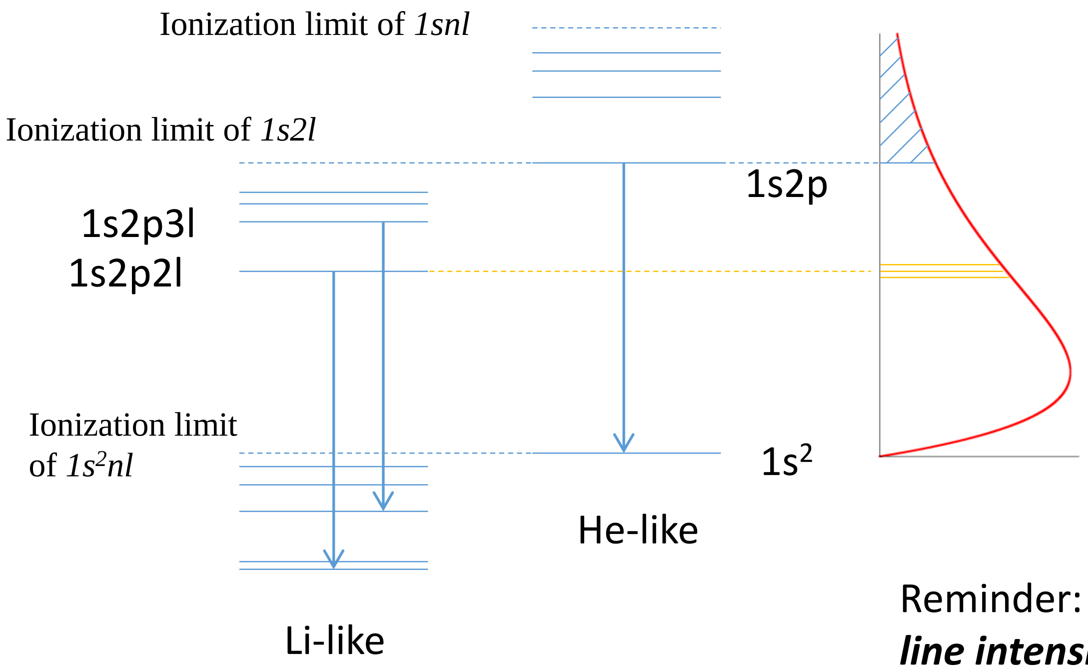
Temperature diagnostics with DS



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

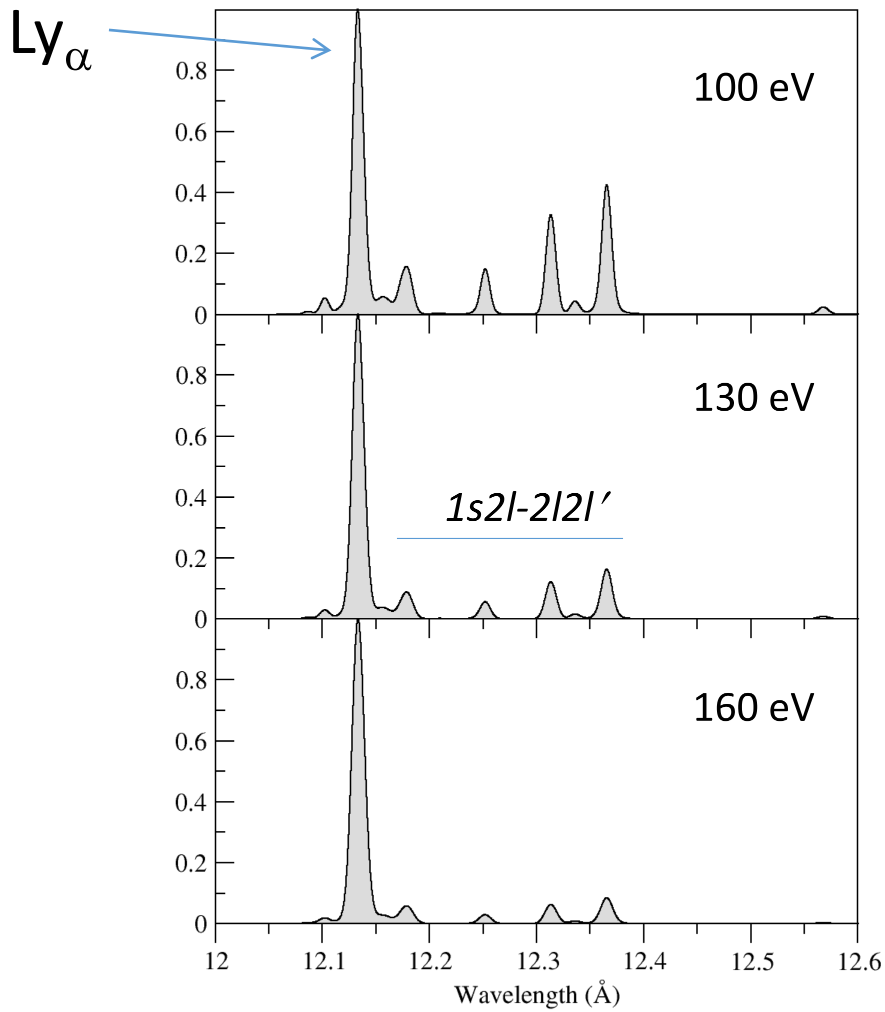
DC rate for 1s2l2l′ ~ $\frac{e^{-\frac{E_s}{T}}}{T^{3/2}}$

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_{α} satellites



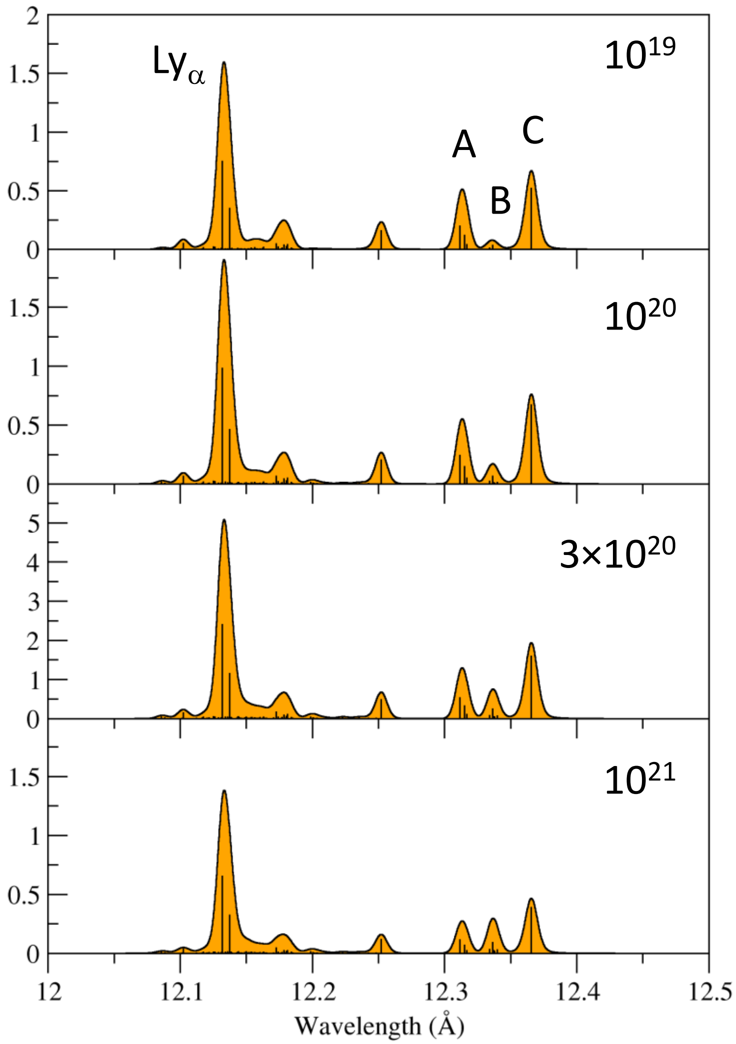
H-like Ne X

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

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

1snl-2l′nl, n=2,3,4,…

Density diagnostics with DS

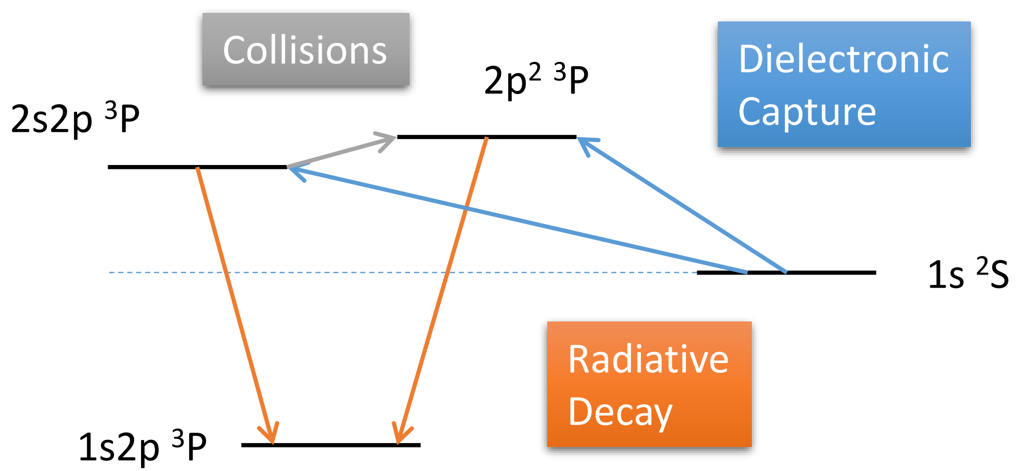


Ne X Ly$_\alpha$ and satellites *1snl-2pnl*

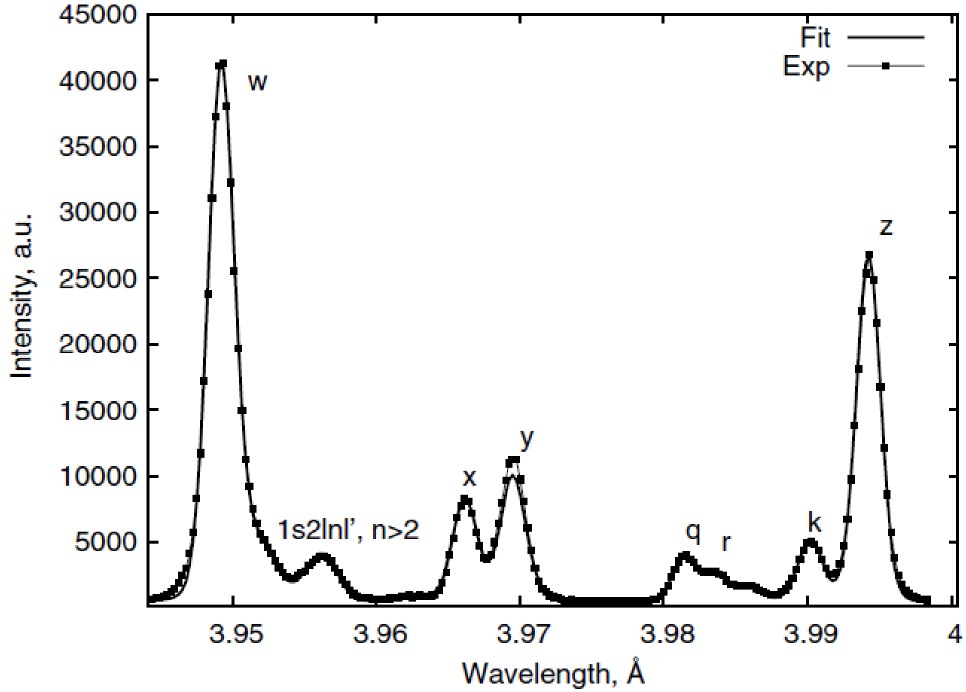
A. 1s2s $^3S_1$ – 2s2p $^3P_{0,1,2}$

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)

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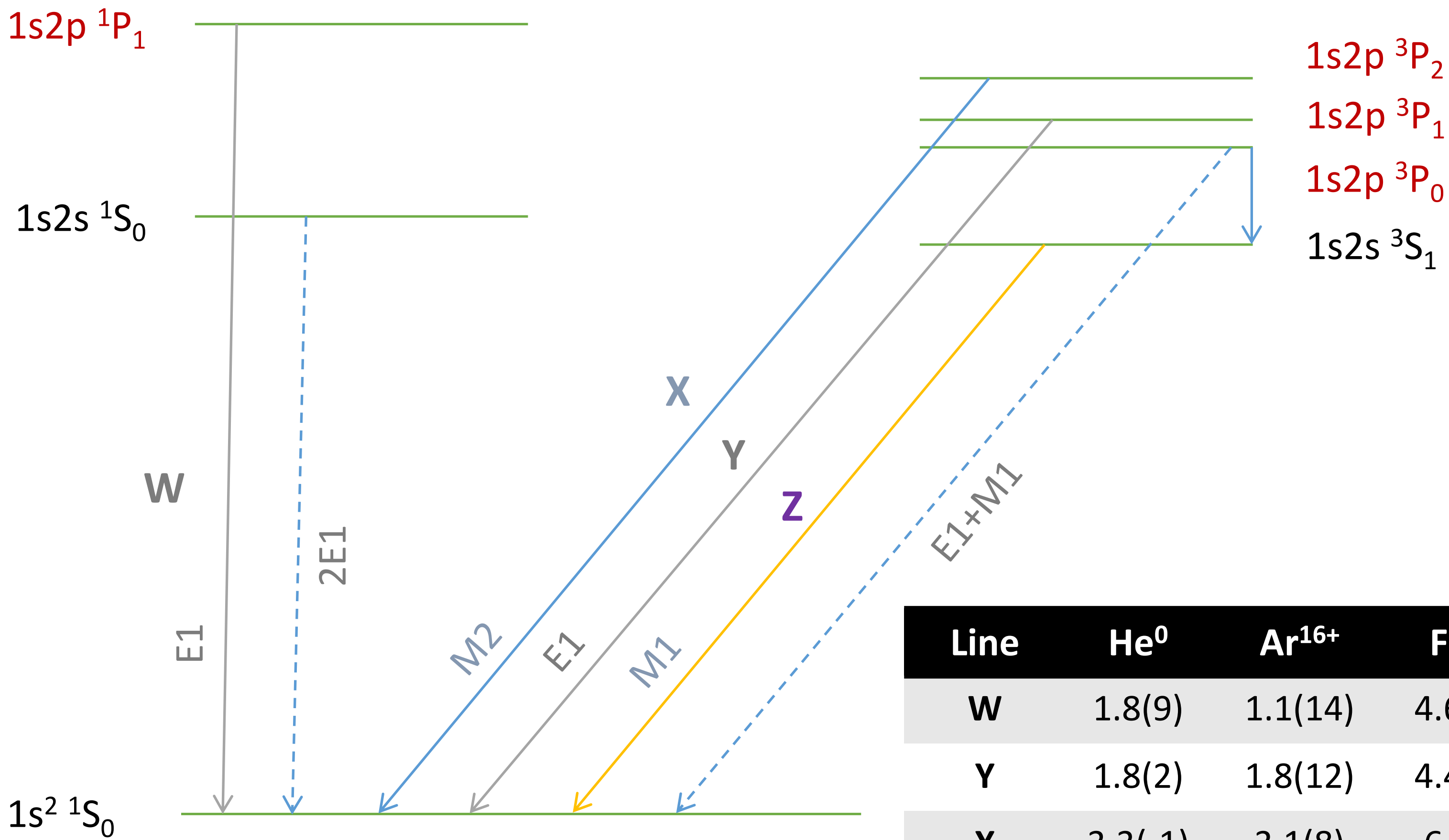
Energy levels in He-like Ar

- 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)

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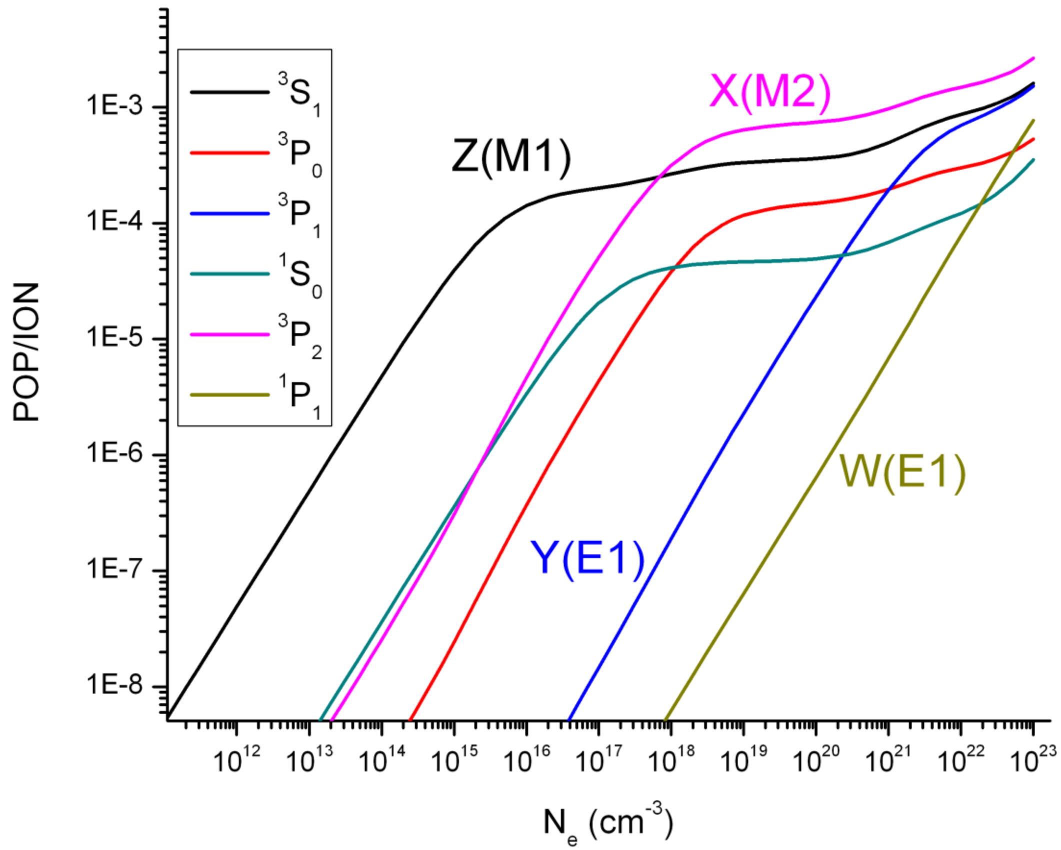
Z-scaling of A's

- 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



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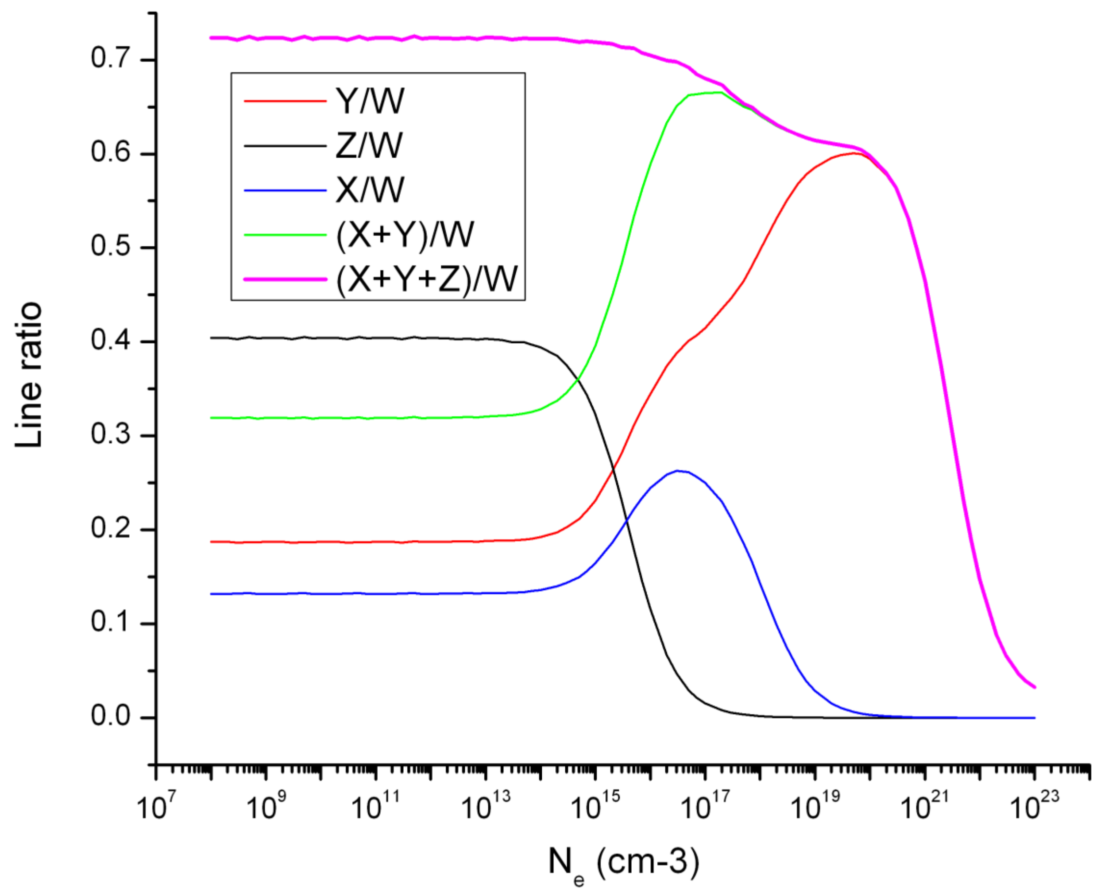
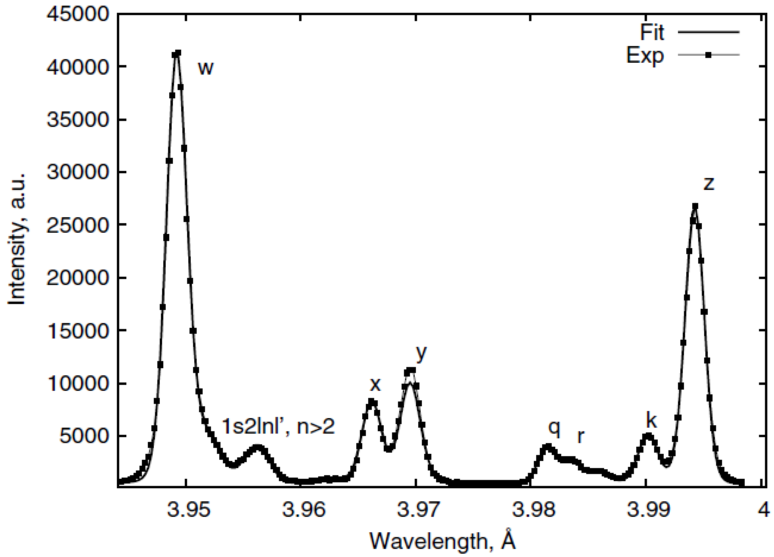
Ar XVII Line Ratios



$1s2lnl$ satellites



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

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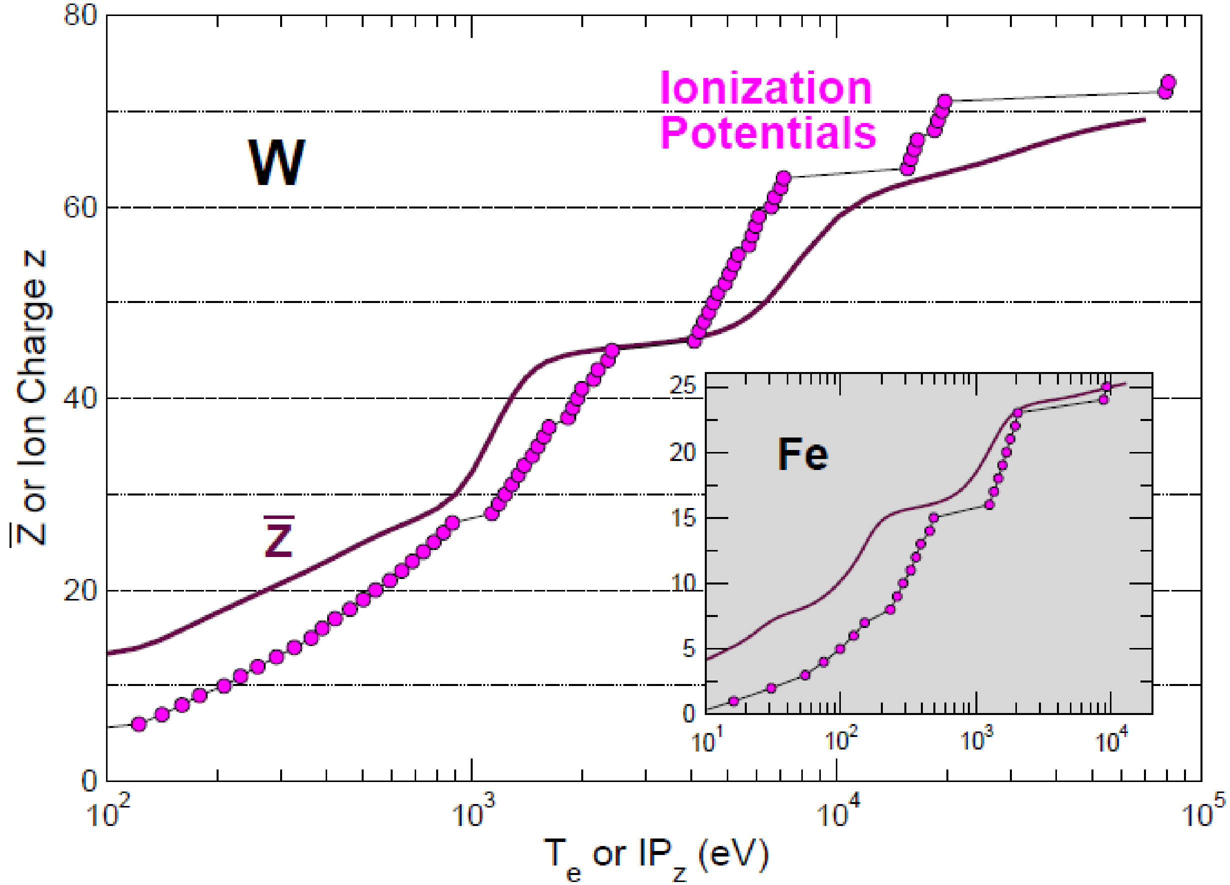
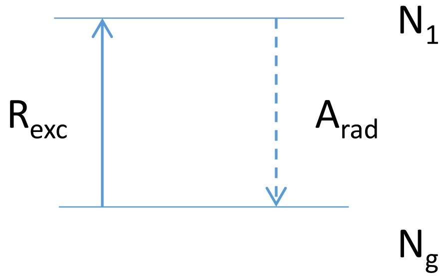
Most Abundant Ions: high Z



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

Time-Dependent Corona



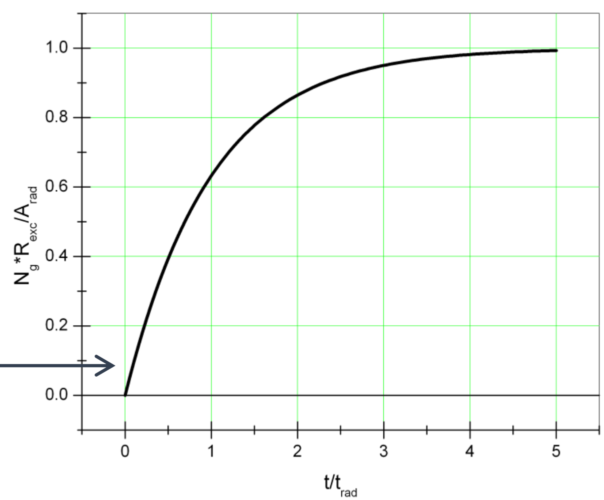
Initial condition: **$N_1(t=0) = 0$**

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

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

Linear regime:

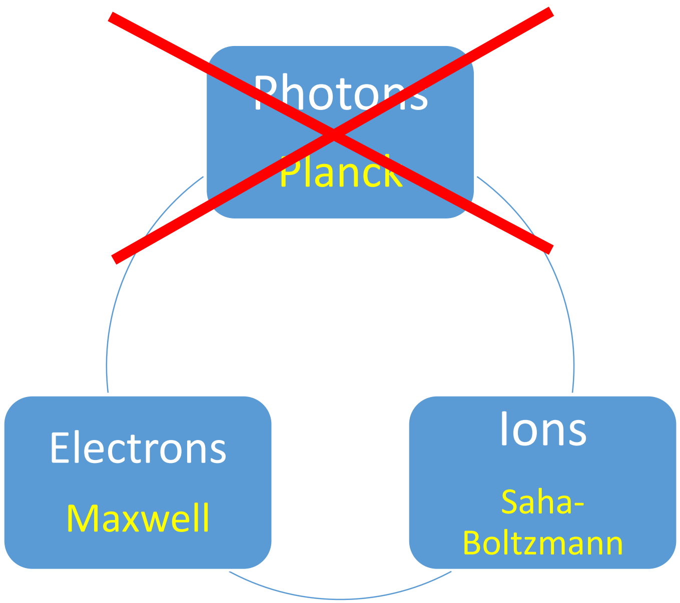
$$N_1(t) \approx N_g R_{exc} t$$

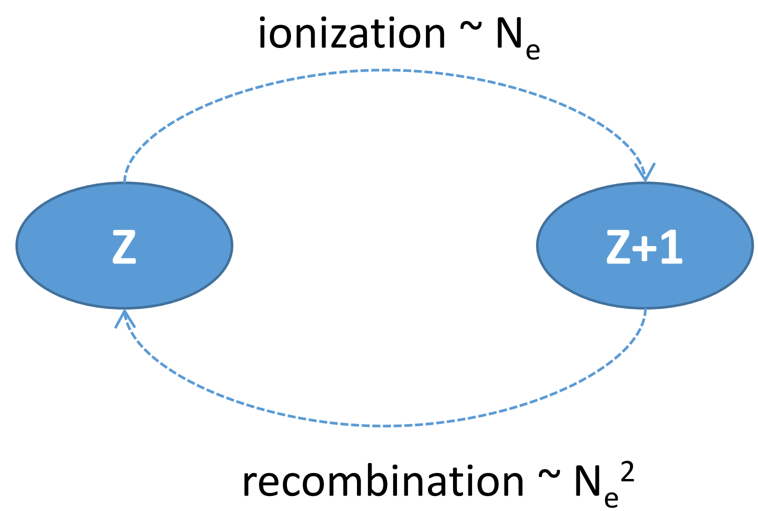


Characteristic time depends only on A_{rad}:

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

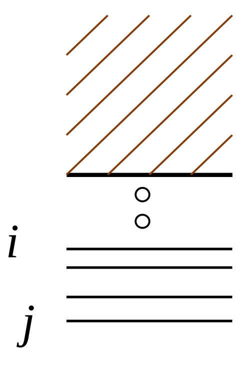
Local thermodynamic equilibrium (LTE)





Saha:

$$\frac{N_{Z+1}}{N_Z} = \frac{1}{N_e}\left(\frac{2\pi T_e}{h^2}\right)^{3/2}\frac{2g_{z+1}}{g_z}\exp\left[-\frac{I_Z}{T_e}\right]$$



Boltzmann:

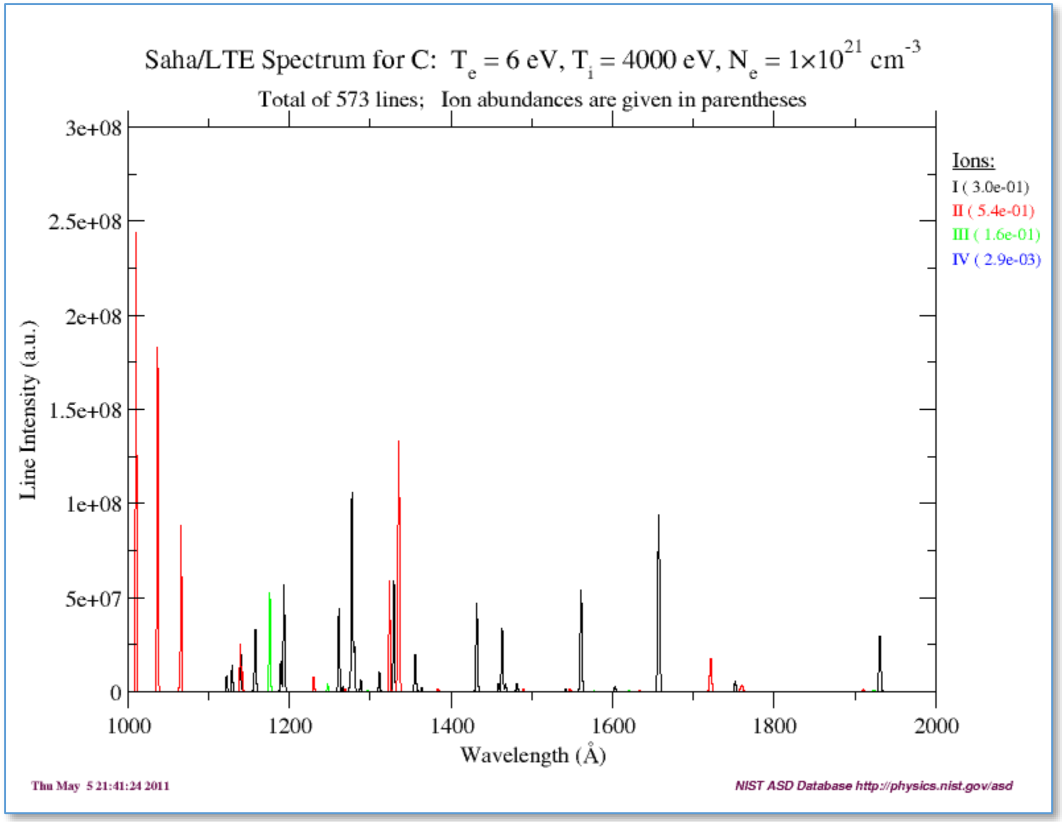
$$\frac{N_i}{N_j} = \frac{g_i}{g_j}\exp\left[-\frac{(E_i - E_j)}{T_e}\right]$$

Collisional processes much stronger than radiative (e.g., N_e is high)

LTE

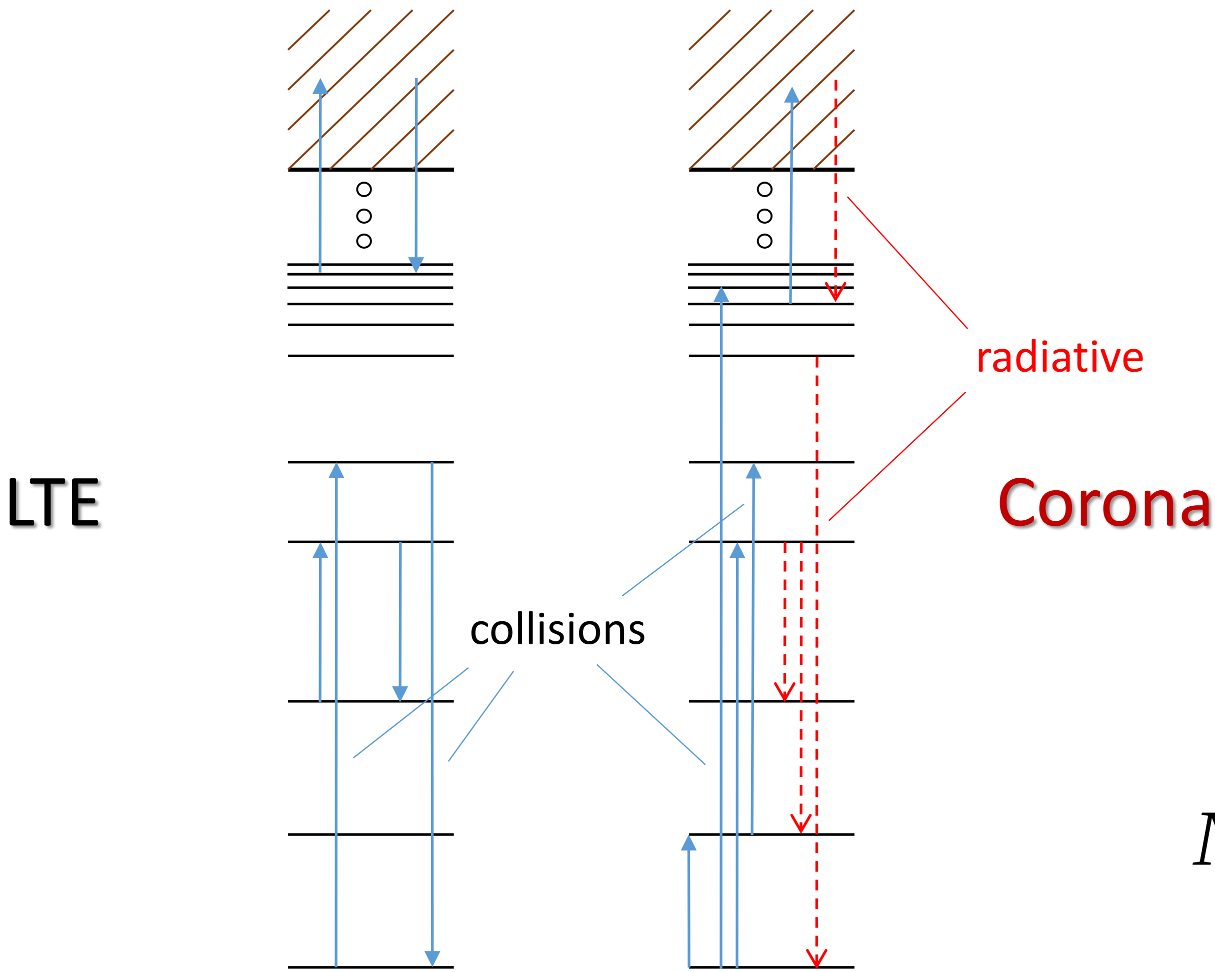
- High densities
  - H: 10^{17} cm^{-3}
  - Ar^{17+}: 10^{25} cm^{-3}
- Does NOT require collisional cross sections, only energy levels (and radiative transition probabilities)
- "statistical" is often used for small energy differences:

$$\frac{N_i}{N_j} = \frac{g_i}{g_j} \exp\left[-\frac{(E_i - E_j)}{T_e} \right]$$



NIST Atomic Spectra Database

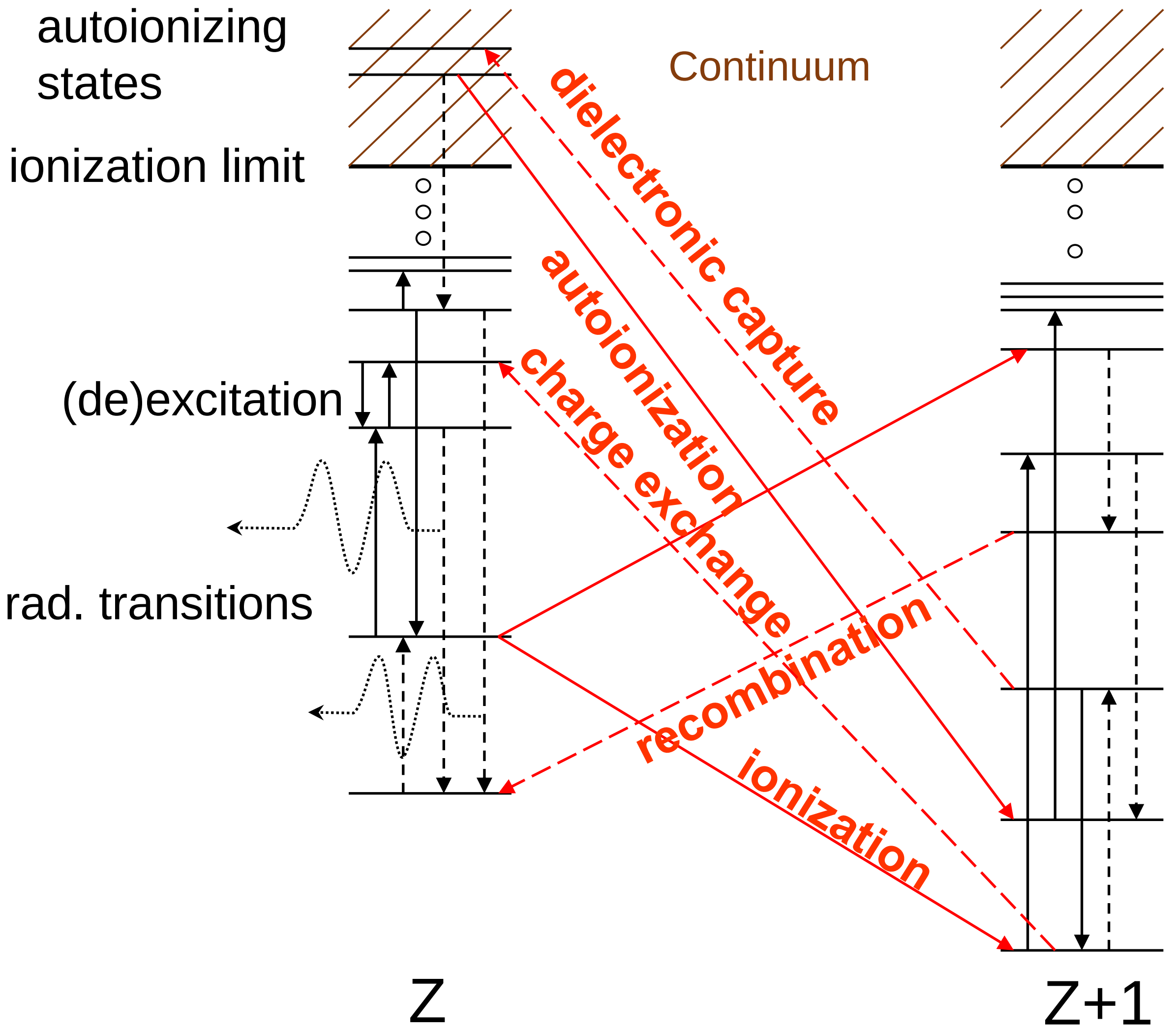
Low N_e: coronal limit



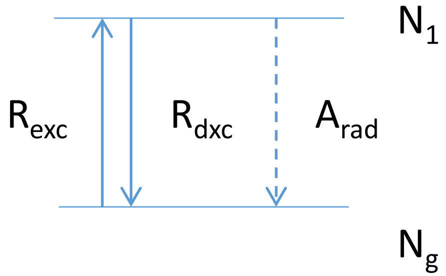
- Excitations (and ionization) only from ground state and metastables
- $A_{rad} \sim N_e^0$, $R_{coll} \sim N_e$ or N_e^2
- Does require a complete set of collisional cross sections
- *Line intensities do not depend on radiative transition probabilities!* (mostly)

$$N_g \cdot R_{gi}^{exc} = N_i \cdot A_{ij}$$

Collisional-radiative modeling of plasma emission



General 2-Level Case



Balance equation:

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

$$\frac{N_1}{N_g} = \frac{R_{exc}}{R_{dxc} + A_{rad}} = \frac{g_1}{g_g}\frac{e^{-\Delta E/T}}{1+W}, \quad W = \frac{A_{rad}}{N_e \langle v\sigma_{dxc}\rangle}$$

Time-dependent case:

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

$$N_g + N_1 = \tilde{N}$$

$$\frac{dN_1(t)}{dt} = \tilde{N}R_{exc} - N_1(t)\left(R_{exc} + R_{dxc} + A_{rad}\right)$$

$$N_1(t) = \frac{\tilde{N}\,R_{exc}}{R_{exc} + R_{dxc} + A_{rad}}\left(1 - e^{-(R_{exc}+R_{dxc}+A_{rad})t}\right)$$

Again at small *t*: $N_1(t) \approx N_g R_{exc} t$

But: $\tau_{eq} \approx \dfrac{1}{R_{exc} + R_{dxc} + A_{rad}}$

Other direct ↔ inverse

- A + e ↔ A^+ + e + e (ionization and 3-body recomb.)

$$g_z\langle v\sigma_i\rangle = 2\left(\frac{mT}{2\pi\hbar^2}\right)^{3/2} g_{z+1}\langle\langle v_1 v_2 \sigma_{3br}\rangle\rangle \exp\left(-\frac{I_z}{T}\right)$$

- A + hν ↔ A^+ + e (photoionization and photorecombination)

$$g_z\sigma_{pi}(h\nu) = \frac{2mc^2E}{h^2\nu^2} g_{z+1}\sigma_{pr}(E), \qquad h\nu = E + I_z$$

Milne formula

Conclusion: only ***direct*** cross sections are sufficient

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