Atomic Processes in Plasmas

A Qualitative Look

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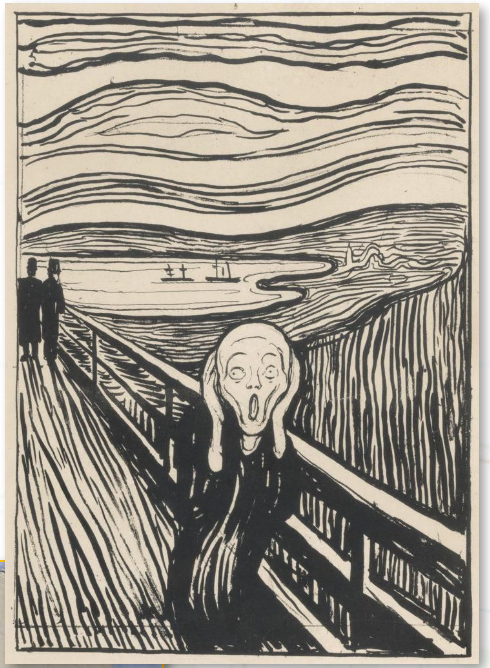
HELP!!!

AFP/Joe Klamar



Question 1: We are building an x-ray laser to hit the asteroid. What is the energy of Ly_α in H-like Ge XXXII?

Question 2: What is its radiative transition probability?

Question 3: What is the excitation cross section/rate coefficient?

Question 4: How hot should the plasma be?

Question 5: What else?..

Energy of Ly_α (eV) in H-like Ge (Z_N=32): take a guess (10 seconds)

$E < 1000$

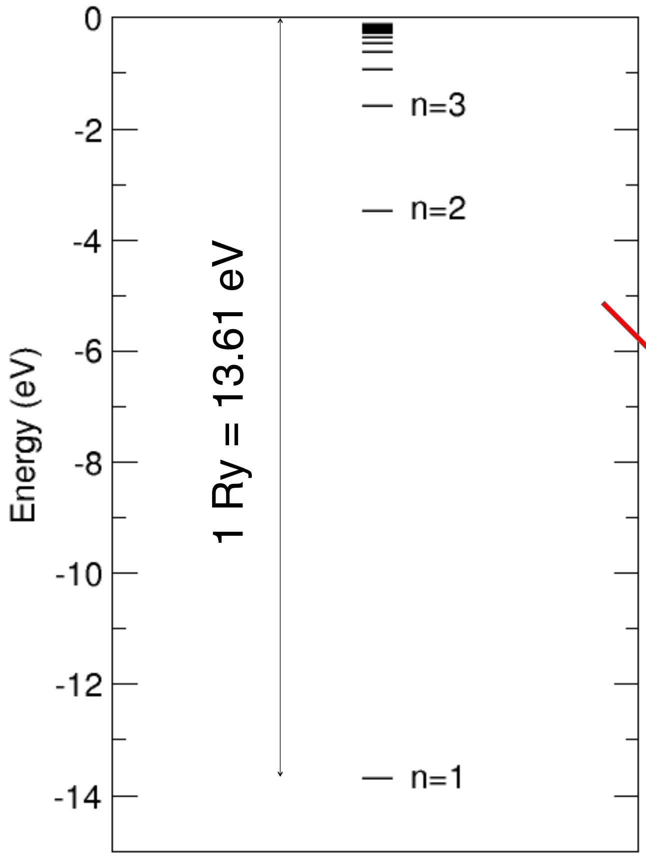
$1000 < E < 5000$

$5000 < E < 9000$

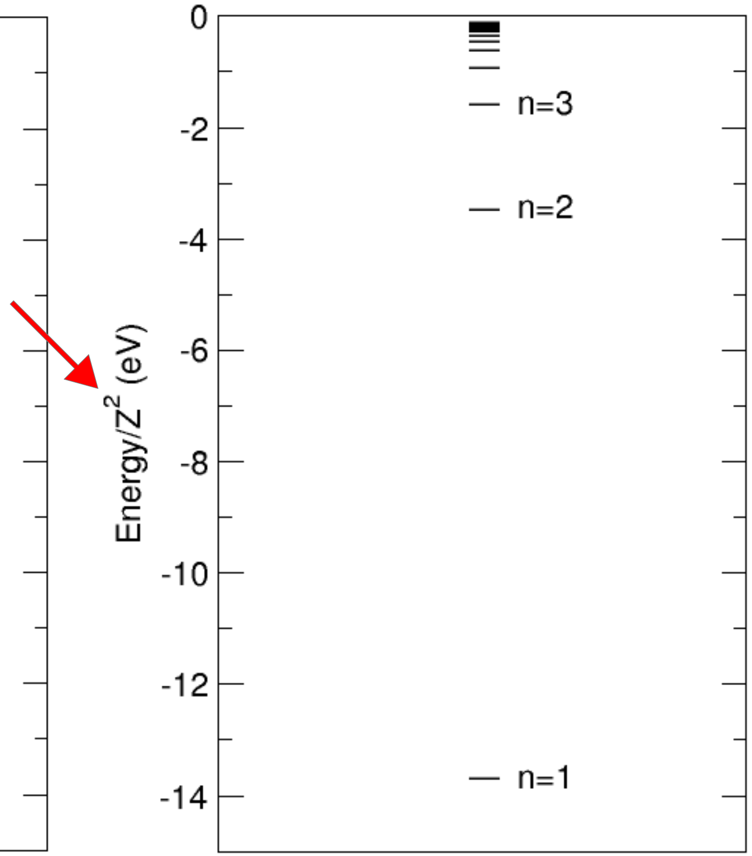
$9000 < E < 12000$

$12000 < E$

NIST ASD: 10,576 eV



Hydrogen atom



H-like ion

Radius: $a_n \sim \frac{n^2}{Z_N}$

Energy: $E_n = -\frac{Z_N^2 Ry}{n^2}$

$$E_{21} = Z_N^2 Ry\left(1 - \frac{1}{2^2}\right) = Z_N^2 Ry \bullet \frac{3}{4}$$

$$E_{21}(Z = 32) \approx 10{,}452\ eV$$

NIST ASD: 10,576 eV

Z_c-scaling of one-electron energies

Spectroscopic charge: **Z_c= ion charge + 1** (H I, Ar XV…)

This is the charge that is seen by the outermost (valence) electron

$$E = E_0 Z_c^2 + E_1 Z_c + E_2 + E_3 Z_c^{-1} + \ldots$$

non-relativistic

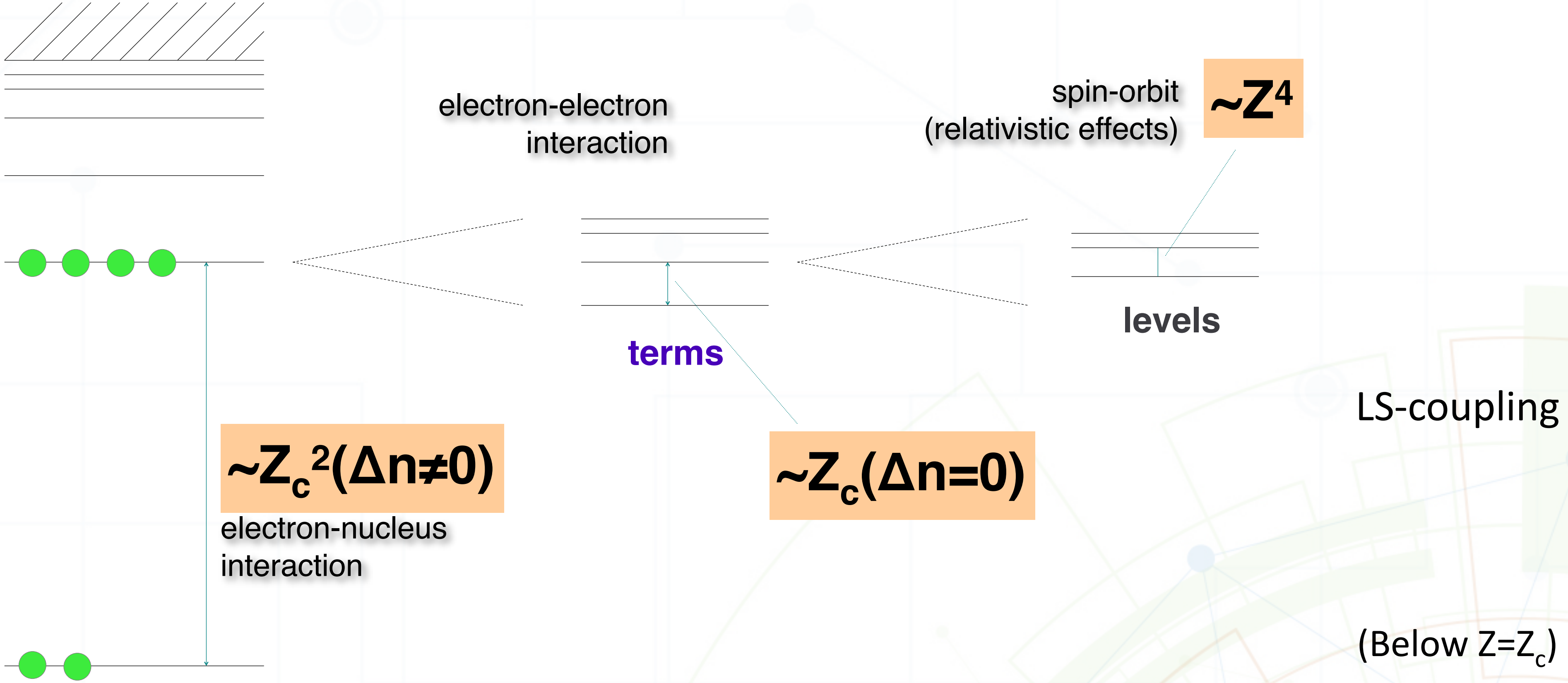
$$E_0 = -\frac{1}{n^2}$$ hydrogenic term

Therefore, for high Z_c the energy structure looks more and more H-like!

K I: $1s^2 2s^2 2p^6 3s^2 3p^6 4s$

W LVI: $1s^2 2s^2 2p^6 3s^2 3p^6 3d$

Of course, relativistic effects slightly modify this dependence
but the general trend remains valid



Every state is defined by a set of quantum numbers which are mostly ***approximate***

Two EXACT quantum numbers:

- ***Parity***
- ***Total angular momentum***

Photons

Positive parity

Negative parity

Quantum electrodynamics: there are two types of photons

Electric 2^J-pole:
Total angular momentum = **J**
Parity = $\mathbf{(-1)^J}$

Electric-dipole E1
Electric-quadrupole E2
Electric-octupole E3
…

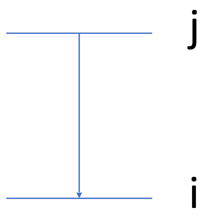
Magnetic 2^J-pole:
Total angular momentum = **J**
Parity = $\mathbf{(-1)^{J+1}}$

Magnetic-dipole M1
Magnetic-quadrupole M2
Magnetic-octupole M3
…

Selection rules

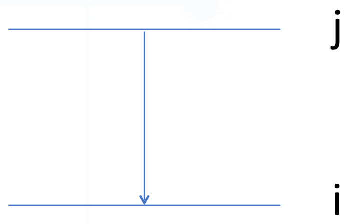
$$P_j = P_i \bullet P_{ph}$$

$$\vec{J}_j = \vec{J}_i + \vec{J}_{ph}$$



E1 is always the strongest (allowed).
Their *transition probabilities* ***A***
strongly decrease with the multipole order.

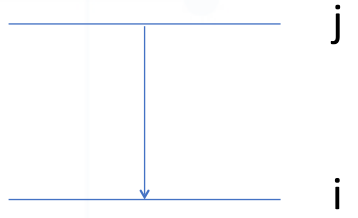
Electric-dipole (E1) transitions



1. Basic matrix element $$\left\langle \Psi_i \middle| r \middle| \Psi_j \right\rangle$$
2. Line strength $$S_{ji} = \left| \left\langle \Psi_i \| r \| \Psi_j \right\rangle \right|^2 = S_{ij}$$
3. Oscillator strength $$f_{ji} = \frac{1}{3g_i} \frac{\Delta E}{Ry} S_{ji}$$ dimensionless — strong lines: 0.1-1
4. Transition probability $$A_{ij} = 4.34 \bullet 10^7 \frac{g_i}{g_j} (\Delta E[eV])^2 f_{ji}$$ [s^{-1}] — neutrals: ~10^8 s^{-1}

E1: Z-scaling

$$a_n \sim \frac{n^2}{Z}$$



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Δn=0	Δn≠0
Z^{-1}	Z^{0}

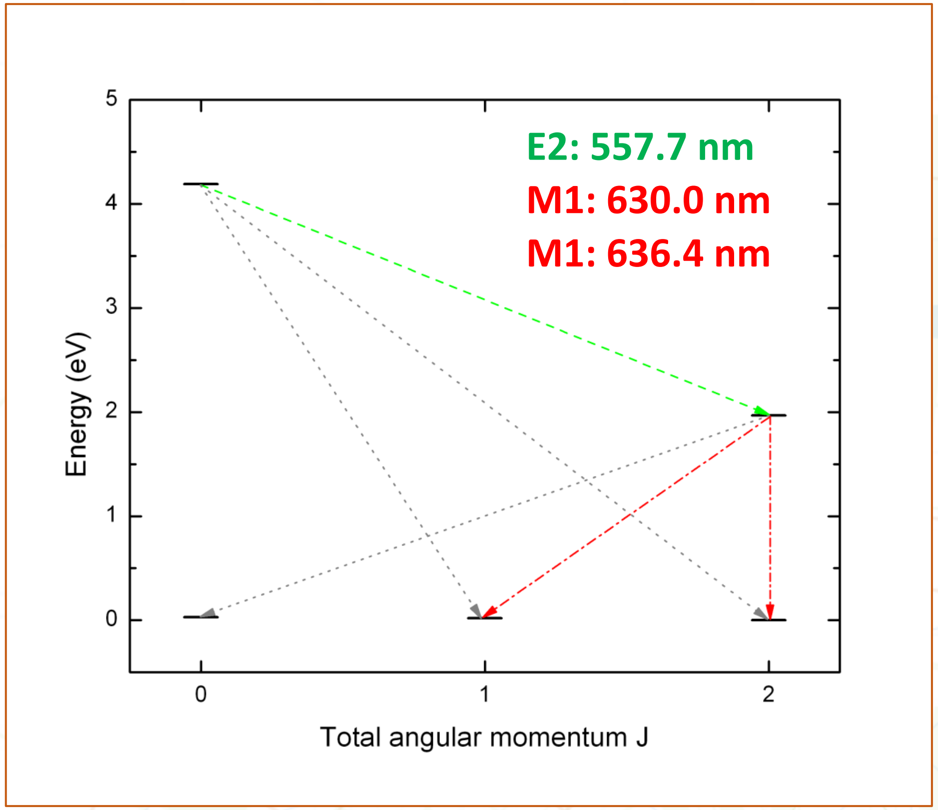
4. Transition probability $A_{ij} = 4.34 \bullet 10^7 \frac{g_i}{g_j} (\Delta E[eV])^2 f_{ji}$

Δn=0	Δn≠0
Z^{1}	Z^{4}

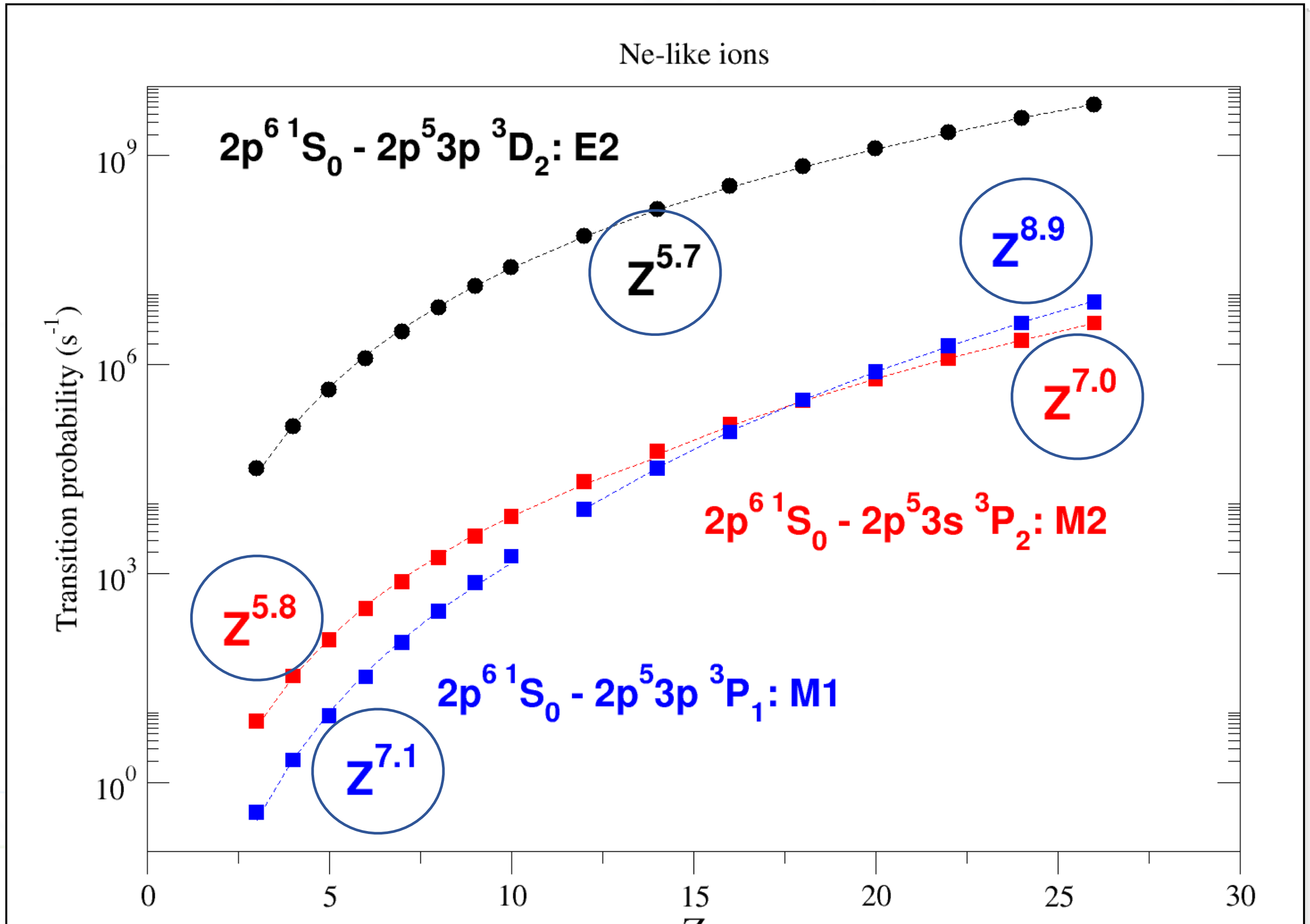
Ly_α in Ge XXXII: ~ $10^8 \times 32^4 \approx 10^{14}$ s^{-1} **NIST ASD: ~6×10^{14} s^{-1}**

Aurora borealis: forbidden transitions in O I

O I $2p^4$



Z-scaling of forbidden transitions: example of Ne-like ions



Jönsson et al, 2014

Ground state:
$1s^2 2s^2 2p^6\ {}^1S_0$

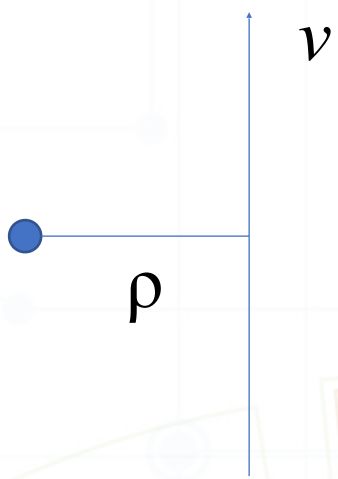
Forbidden transitions become more and more important with Z relative to allowed transitions

Collisions

- Cross sections are *probabilities*
  - Classically: $\sigma(\Delta E, E) = \int_0^\infty P(\Delta E, E, \rho) \cdot 2\pi\rho d\rho$
- Typical values for atomic cross sections
  - $a_0 = 5.29 \cdot 10^{-9}$ cm $\Rightarrow \pi a_0^2 \sim 10^{-16}$ cm^2
- 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



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

Examples in He I:

$1s^2\ ^1S \rightarrow 1s2p\ ^1P$
$1s2p\ ^3P \rightarrow 1s4d\ ^3D$

$1s2s\ ^1S \rightarrow 1s3s\ ^1S$
$1s2s\ ^3S \rightarrow 1s4d\ ^3D$

$1s^2\ ^1S \rightarrow 1s2p\ ^3P$
$1s2p\ ^3P \rightarrow 1s4d\ ^1D$

Van Regemorter-Seaton-Bethe formula

- <u>Optically-allowed</u> 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: $g(X)$

oscillator strength: f_{ij}

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

$$\sigma_{ij}(E) \propto \frac{f}{\Delta E_{ij}^2}$$

Z-Scaling of Excitations

$$\sigma_{ij}(E) \propto \frac{f}{\Delta E_{ij}^2}$$

Δn=0

- $f \sim Z^{-1}$, $\Delta E \sim Z$, **$\sigma \sim Z^{-3}$, $\langle v\sigma \rangle \sim Z^{-2}$**

Δn≠0

- $f \sim Z^{0}$, $\Delta E \sim Z^{2}$, **$\sigma \sim Z^{-4}$, $\langle v\sigma \rangle \sim Z^{-3}$**

If for neutrals $\sigma \sim 10^{-16}$ cm^2 and $v \sim 10^8$ cm/s (a.u.), then $\langle \sigma v \rangle \sim 10^{-8}$ cm^3/s

For H-like Ge XXXII ~ 3×10^{-13} cm^3/s

Maxwellian rate coefficient for Ge XXXII 1s-2p excitations

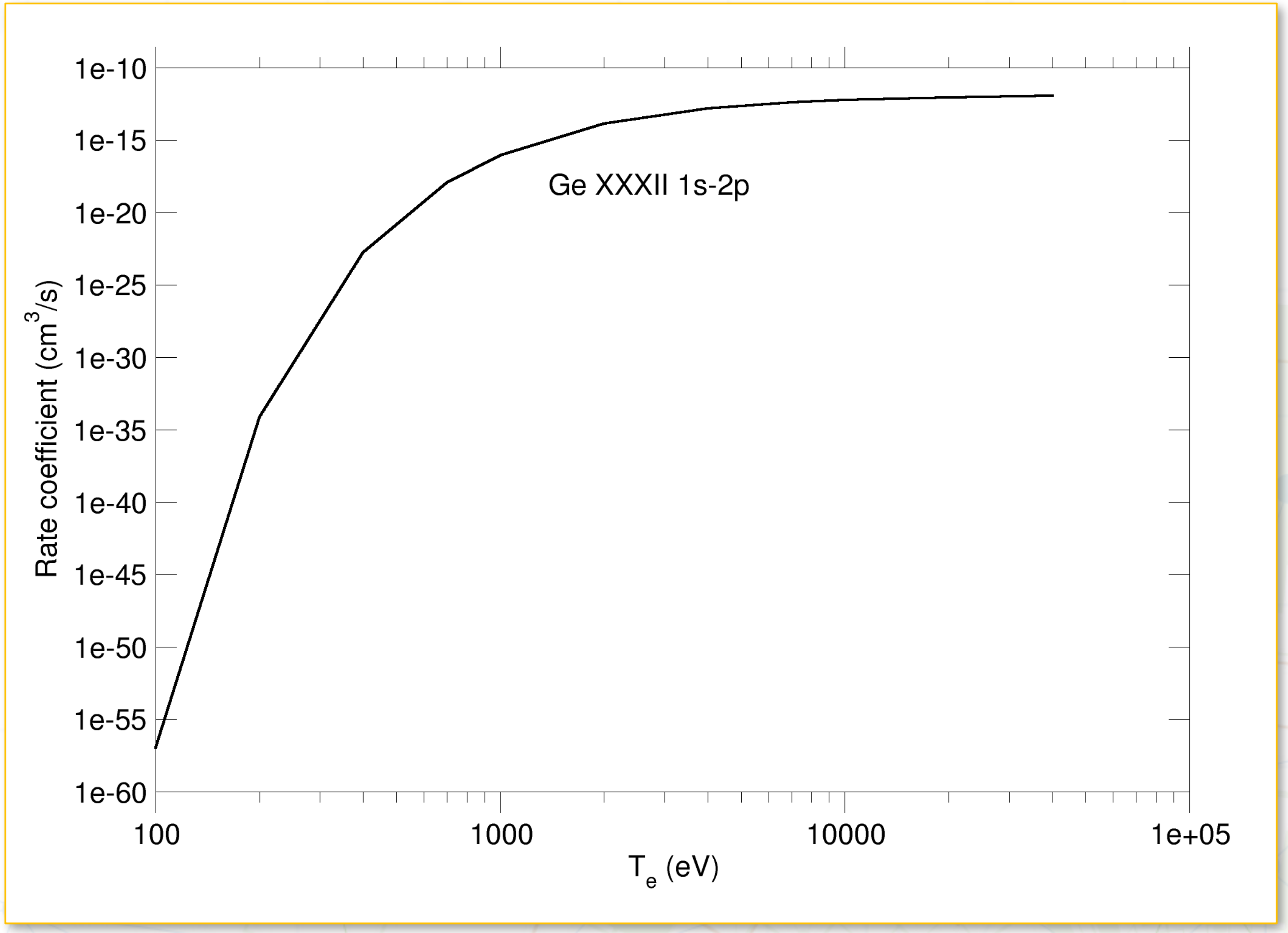
$$\langle \sigma v \rangle = \left(\frac{8}{\pi m T^3} \right)^{1/2} \int_{\Delta E}^{\infty} E \bullet \sigma(E) \bullet e^{-E/T} dE$$

For $\sigma(E) = A/E$: $\langle v\sigma \rangle \propto \frac{e^{-\frac{\Delta E}{T}}}{\sqrt{T}}$

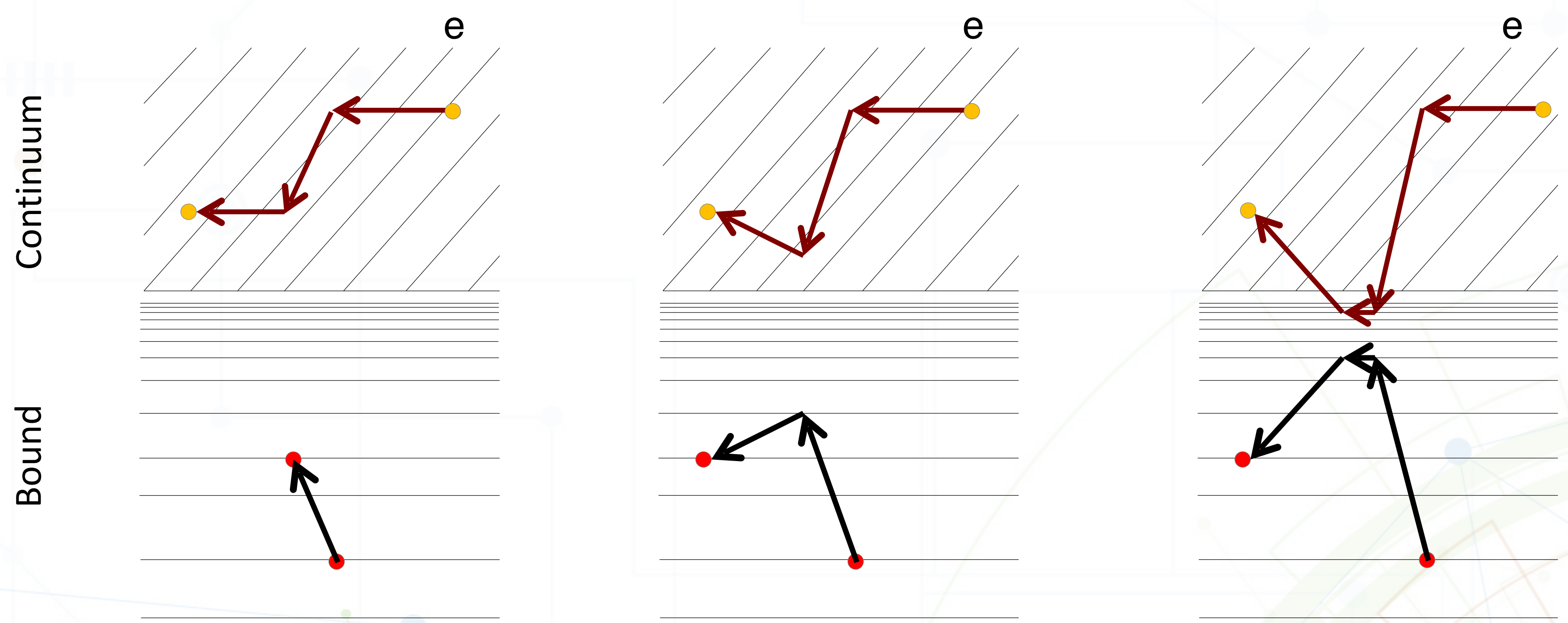
Estimate:

For H-like Ge XXXII ~ 3×10^{-13} cm^3/s

Flexible Atomic Code (M.F. Gu)



Resonances in excitations



Direct excitation | Intermediate states | Intermediate AI states

Autoionization

- Examples of AI states
  - $1s2s^2$, 2l2l\`, $1s^22pnl$ (high n)
- Same old rule: **before = after**
- $A^{**} \rightarrow A^* + \varepsilon l$
  - ***Exact***: $P_j = P_i$; $\Delta J = 0$
  - *Approximate* (LS coupling): **$\Delta S = 0$, $\Delta L = 0$**

P=+1

- $2p^2\ ^1S_0 \rightarrow 1s + \varepsilon s$: *good*
- $2p^2\ ^1D_2 \rightarrow 1s + \varepsilon d$: *good*

- $2p^2\ ^3P_{0,1,2} \rightarrow 1s + \varepsilon p$: *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: $A_a(2p^2\ ^3P_1) \approx 0$

A_a are typically on the order of 10^{13}-10^{14} s^{-1} and they (almost) do not depend on Z_c

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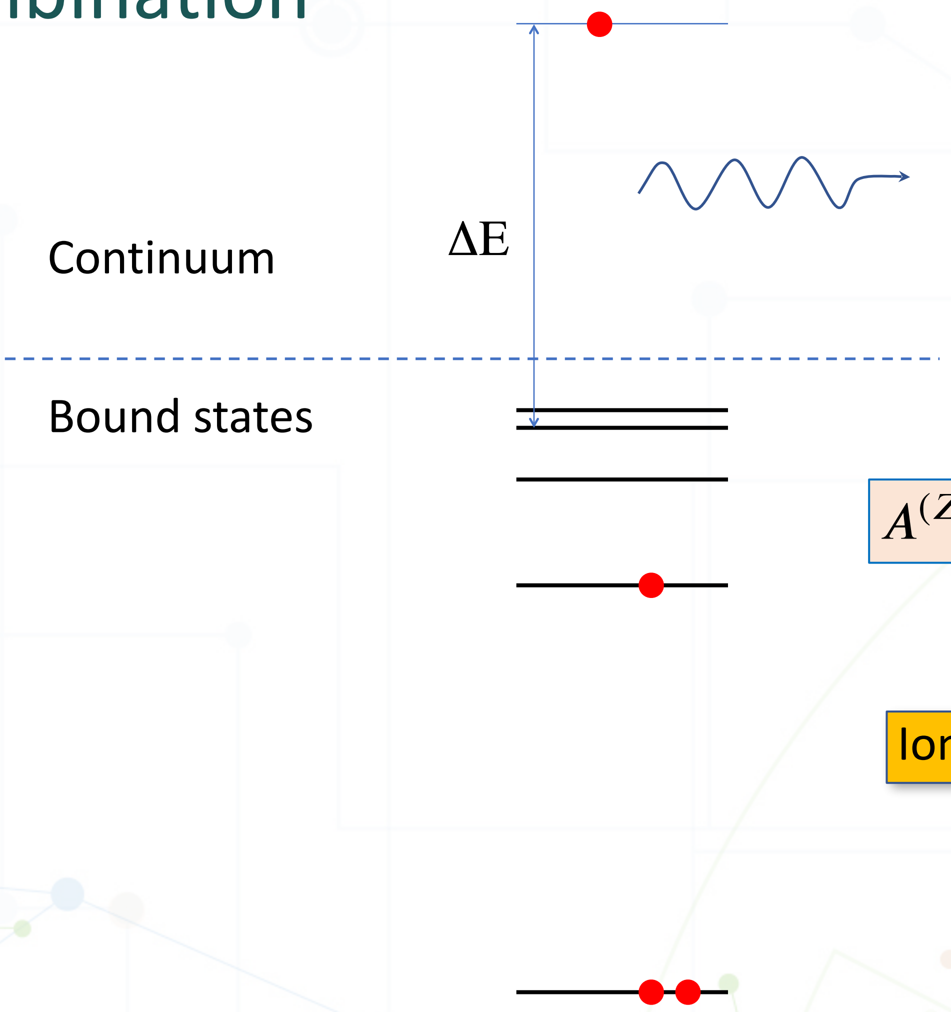
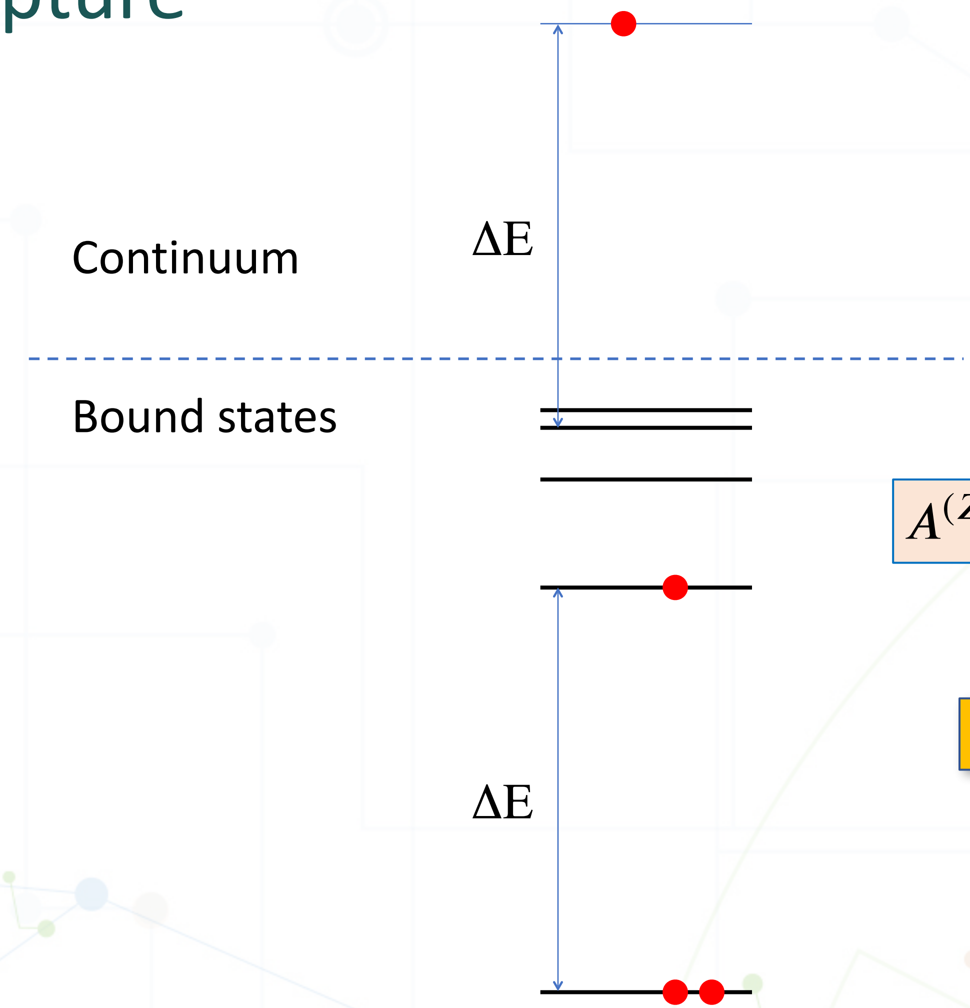
Radiative recombination



$$A^{(Z+1)+} + e \rightarrow A^{Z+} + h\nu$$

Ion recombined

Dielectronic capture

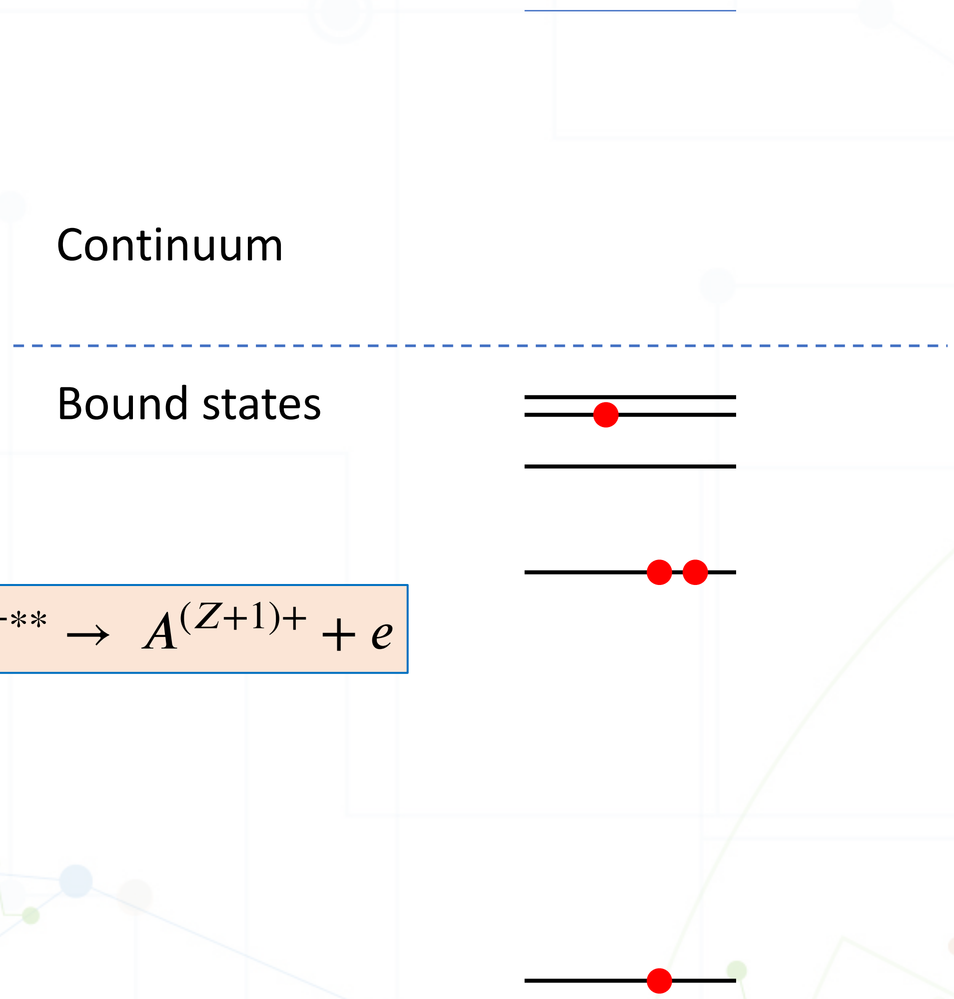


$$A^{(Z+1)+} + e \rightarrow A^{Z+**}$$

Resonant process!

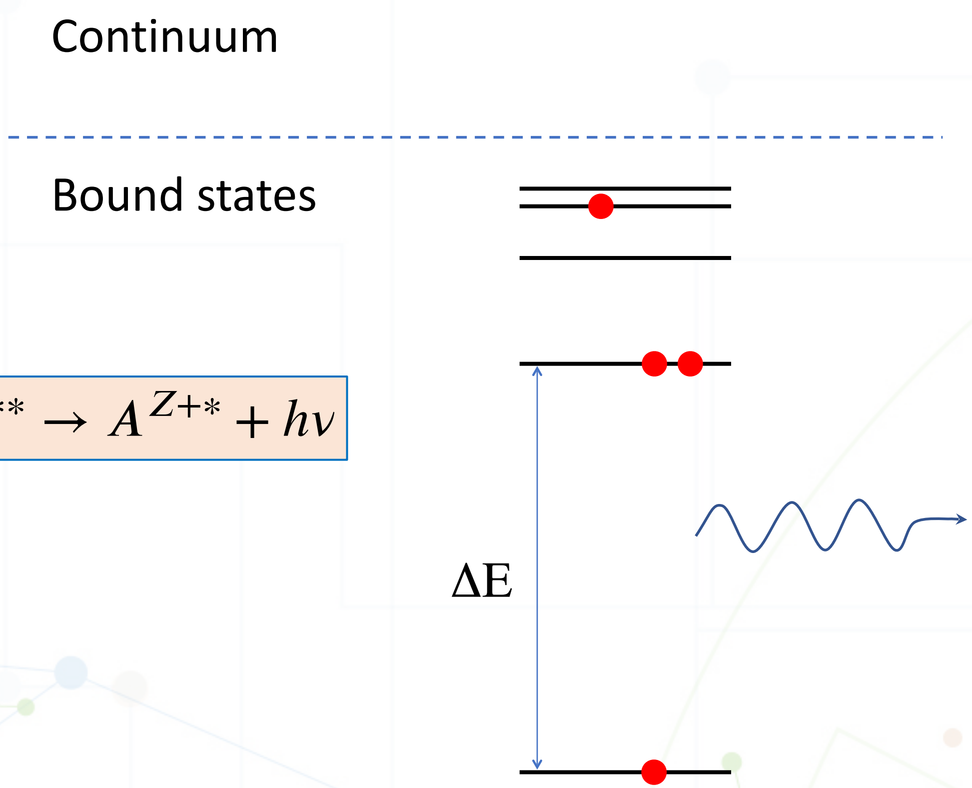
DC ←→ AI

DC and AI are
direct and inverse



$$A^{(Z+1)+} + e \rightarrow A^{Z+**} \rightarrow A^{(Z+1)+} + e$$

Dielectronic recombination = DC + radiative stabilization



$$A^{(Z+1)+} + e \rightarrow A^{Z+**} \rightarrow A^{Z+*} + h\nu$$

$$\Delta E(\Delta n = 0) \propto Zc$$

$$\Delta E(\Delta n \neq 0) \sim 13.6eV \bullet Zc^2$$

Stabilizing transition:
Mostly x-rays

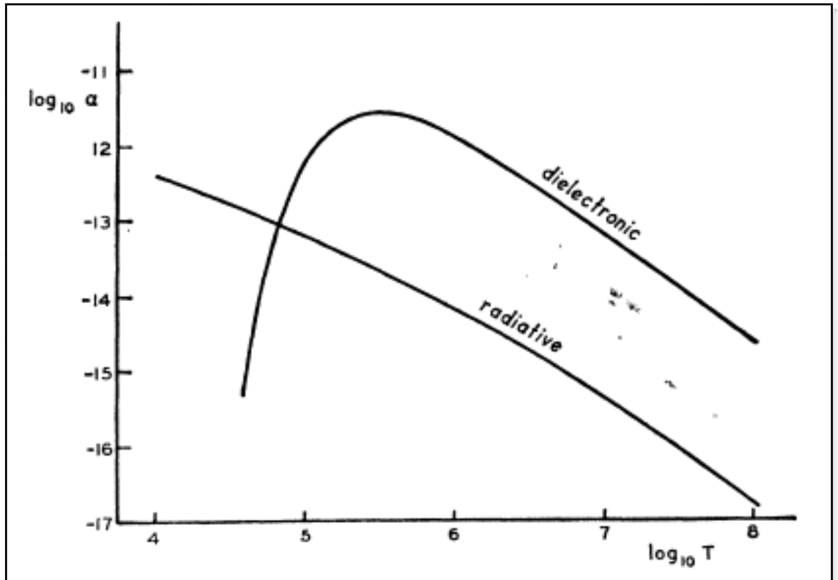
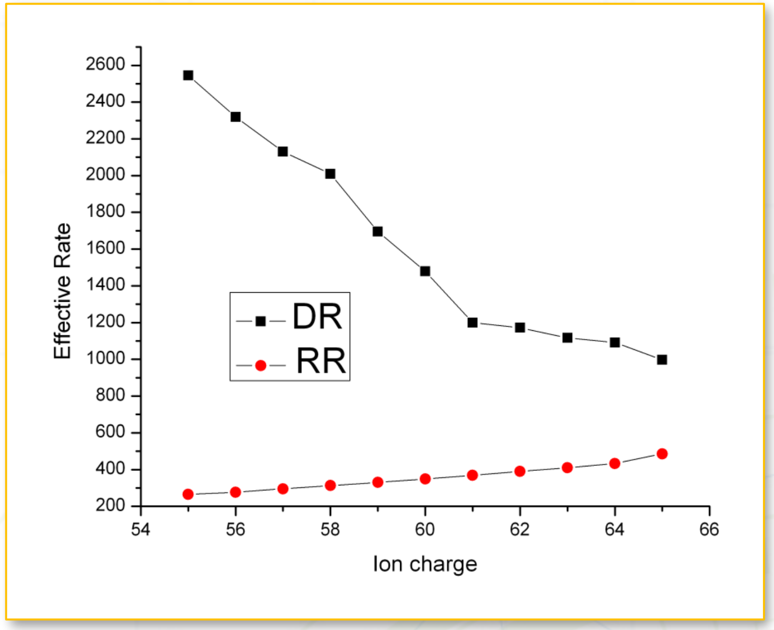


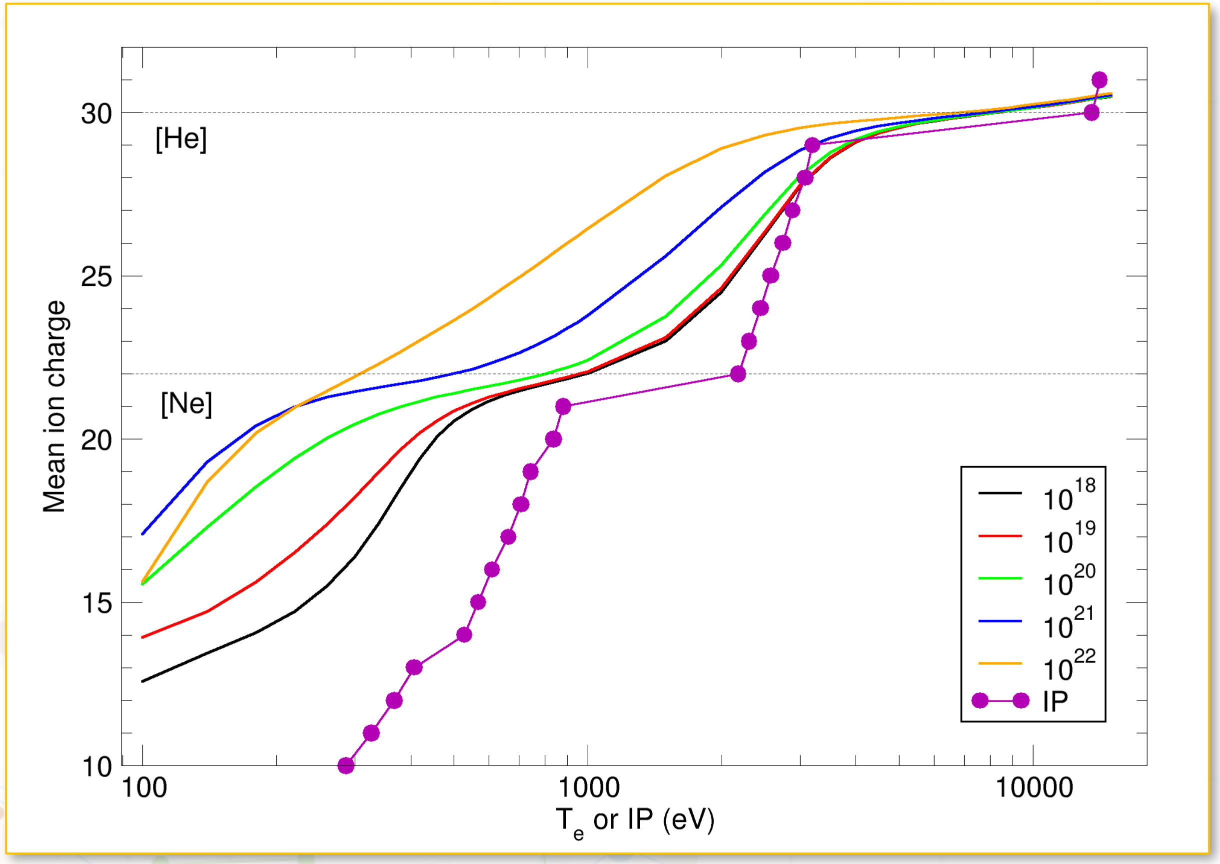
FIG 1.—He⁺ + e recombination coefficients α (cm³ sec⁻¹)

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

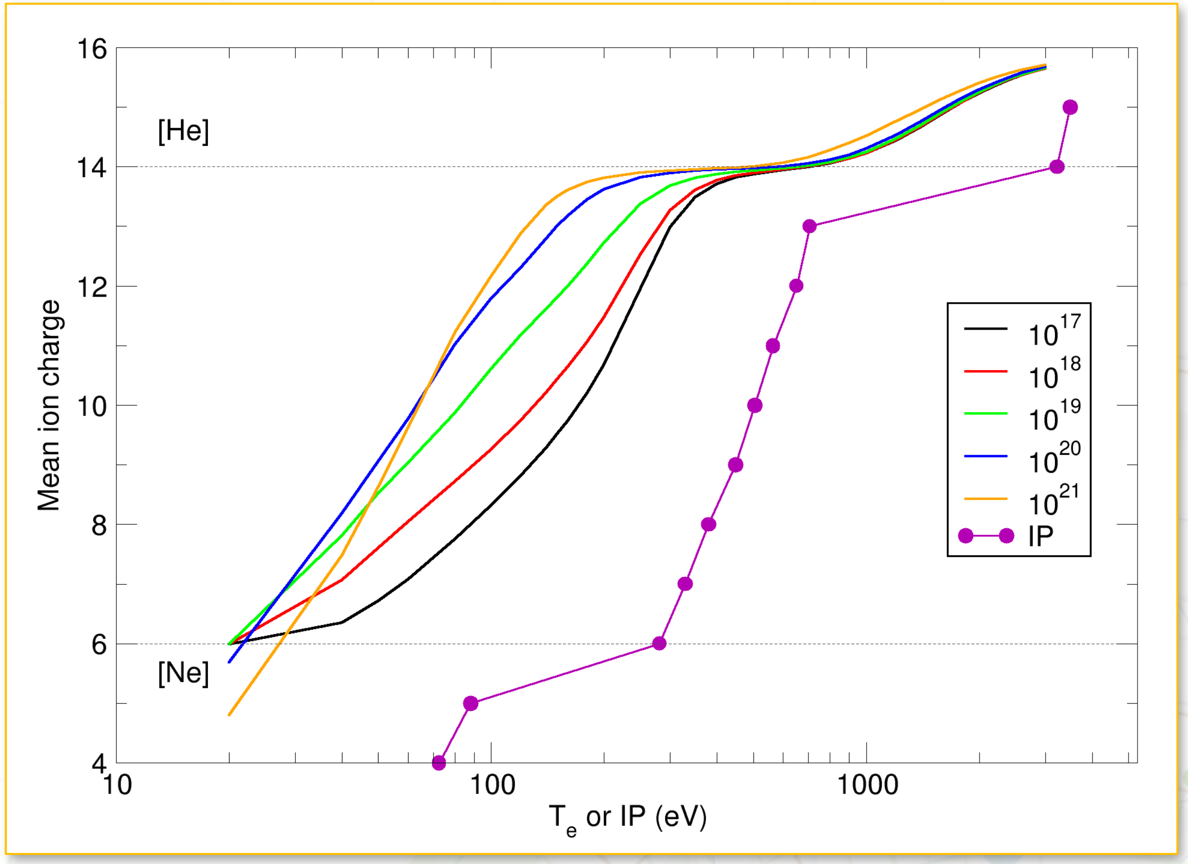


W at 9 keV, 10^{14} cm^{-3}

Ge (Z=32)



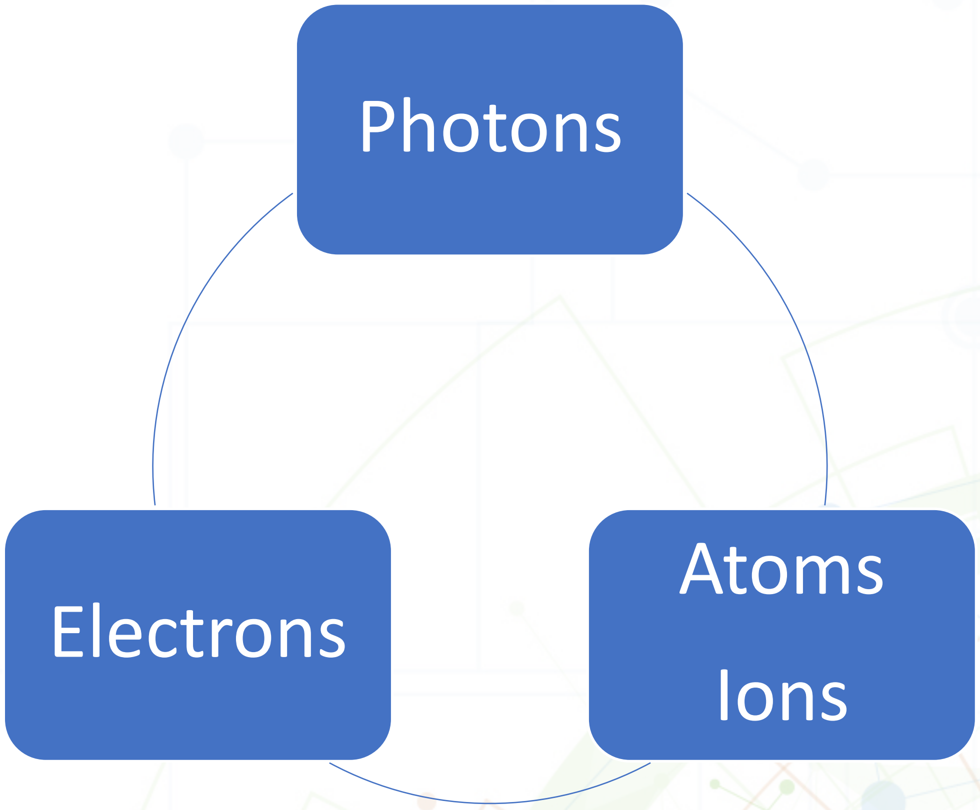
S (Z=16)



FLYCHK: https://nlte.nist.gov/FLY

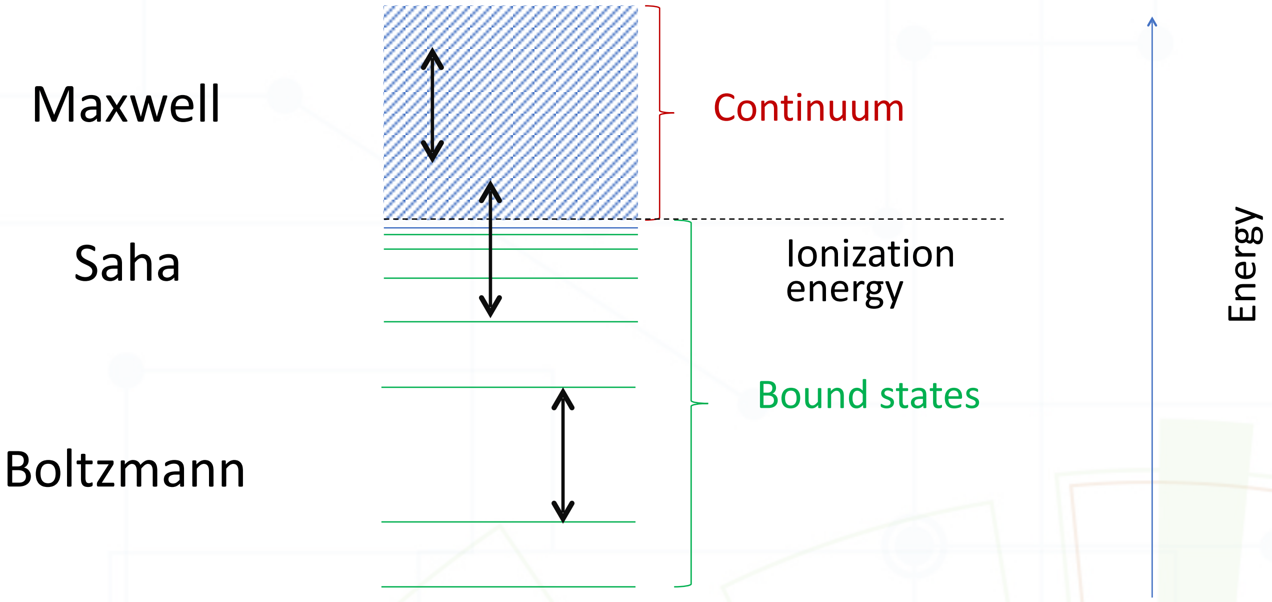
Thermodynamic Equilibrium

- 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

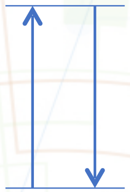


TE distributions

- 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



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



But: photons are easily decoupled…no complete TE

Local Thermodynamic Equilibrium (high N_e, low T_e)

- LTE = Saha + Boltzmann + Maxwell
- ***No atomic data*** (only energies and statweights) are needed to calculate populations, A's needed for line intensities
- Griem's criterion for Boltzmann: *collisional rates > 10*radiative rates*

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

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

Saha:

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

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

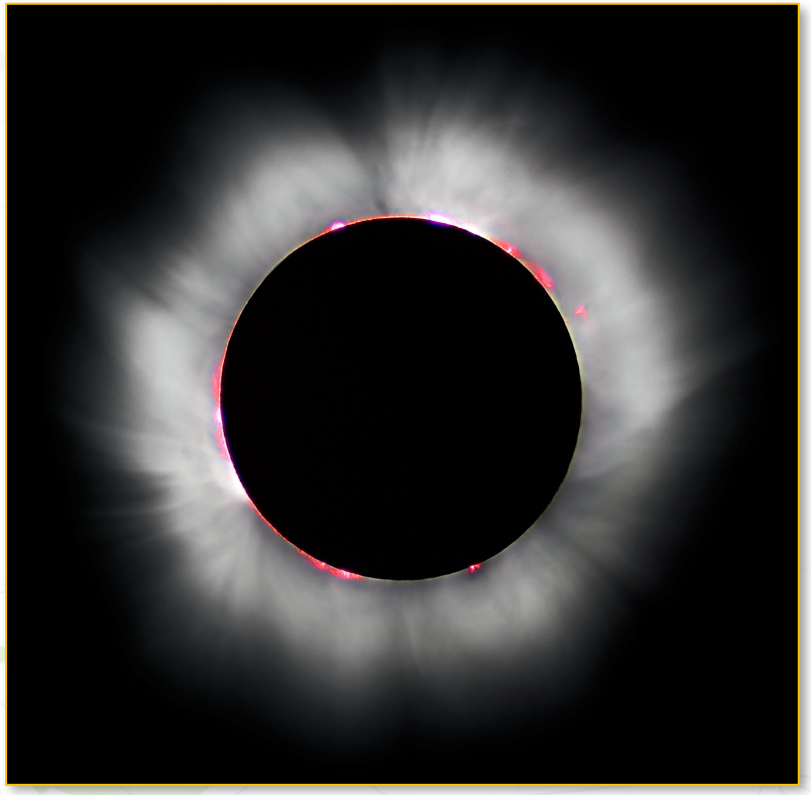
$$\Rightarrow \quad \frac{N^{Z+1}}{N^Z} = 1 \qquad \frac{I_Z}{T_e} >> 1\left(\sim 10\right)$$

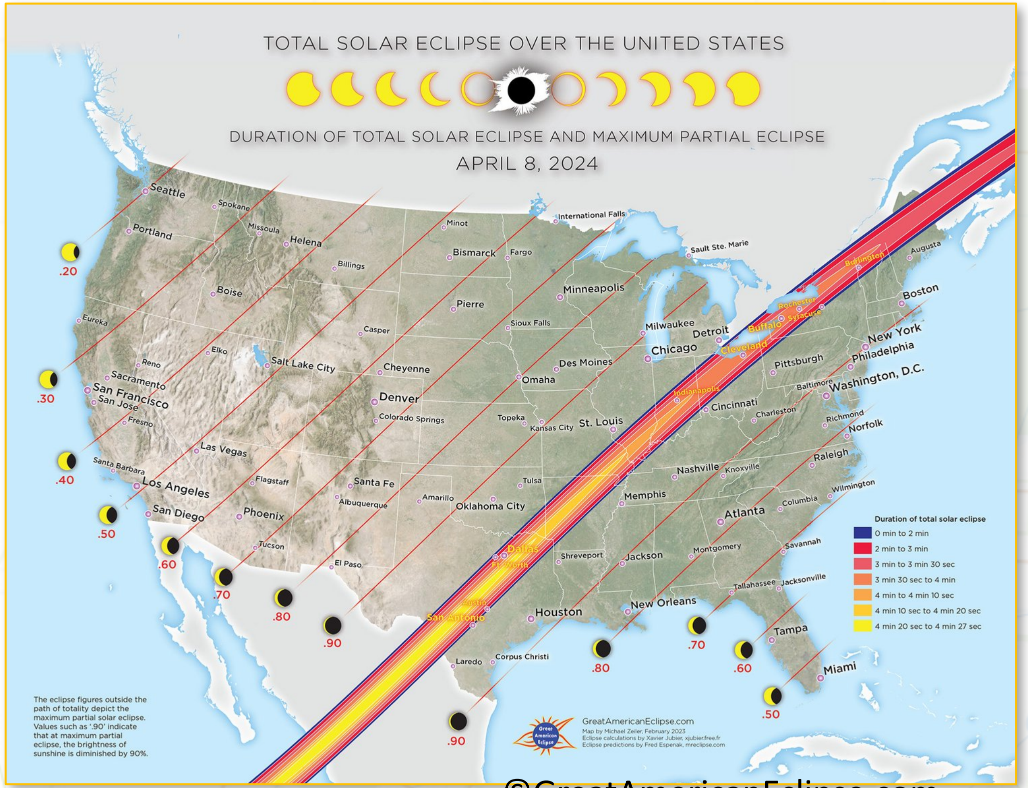
Coronal Equilibrium (high T_e, low N_e)

Does require a complete set of collisional cross sections and A values

Ionization balance does NOT depend on N_e ($I_z/T_e \sim 3$)

Next big: Apr 8, 2024





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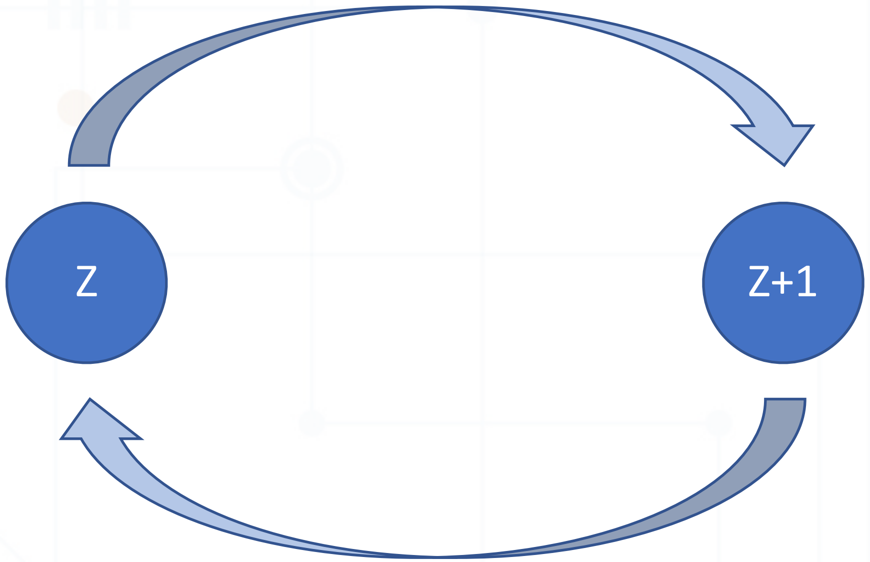
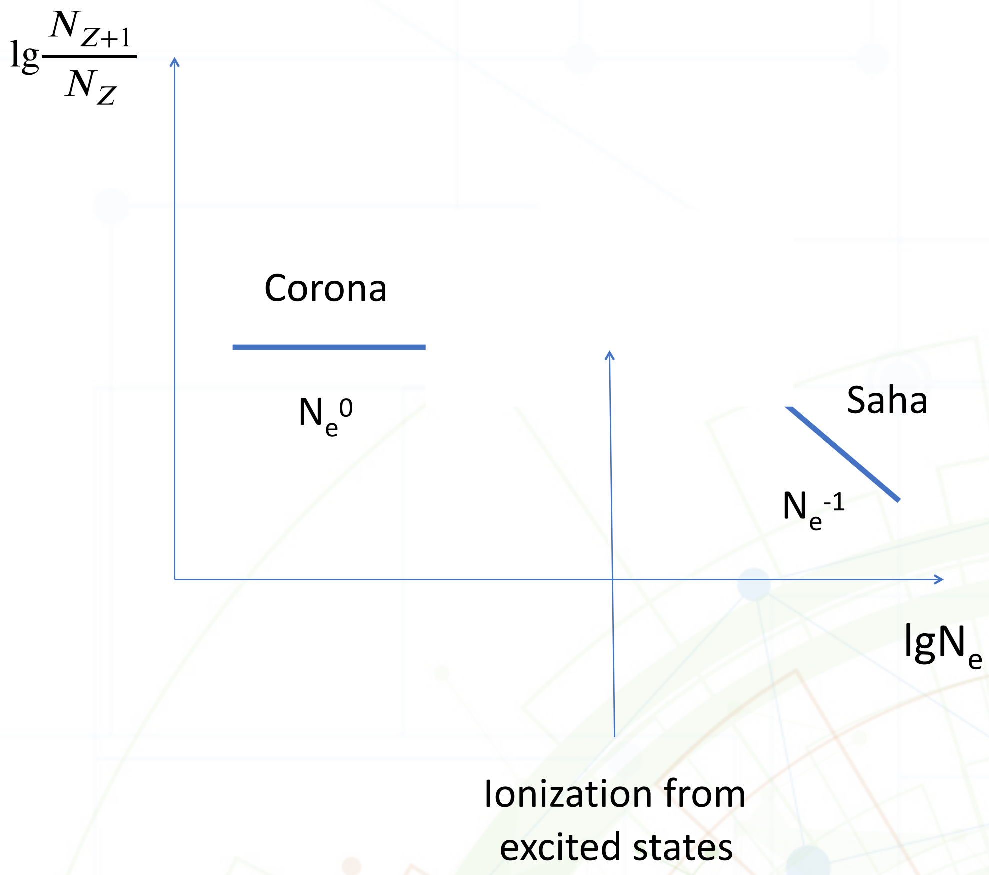
Electron-impact ionization: N_e



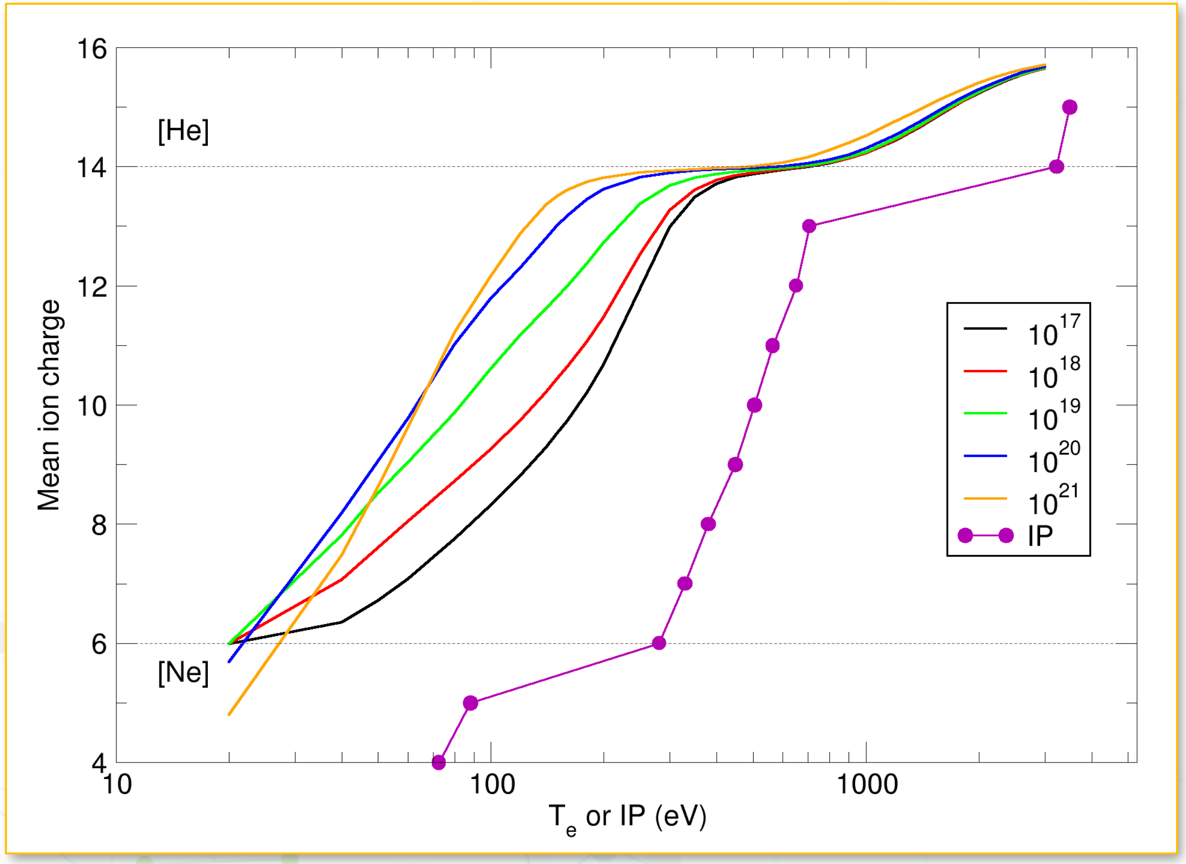
Photorecombination and DR: $\propto N_e$

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

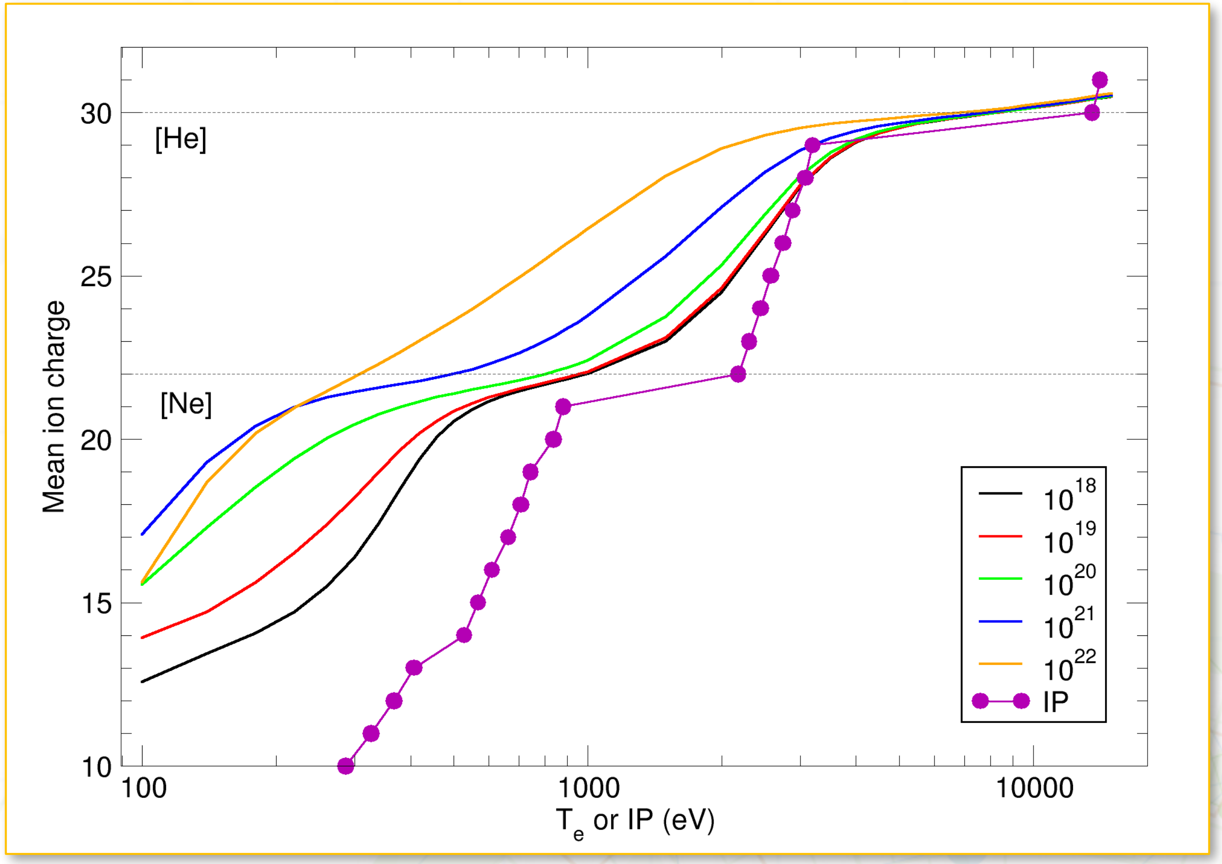
Ratio of ion populations



S (Z=16)



Ge (Z=32)



FLYCHK: https://nlte.nist.gov/FLY

Conclusions

- Many characteristics of atomic processes in plasmas can be estimated using simple qualitative methods
- Use them!