Atomic Data for Plasmas:
Structure, Radiation, Collisions

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Few notes

- Not a complete course on A&M data for plasmas
- Don't feel discouraged if you see something familiar (you certainly will)
- Ask questions
- Talk with the other students
- Talk with the lecturers

What is this about?..

- Most general overview of atomic parameters that are relevant to plasma spectroscopy
- Qualitative estimates
- Selection rules
- Scalings
- …

A Few Textbooks on Atomic Physics/Plasma Spectroscopy

R.D. Cowan

Theory of Atomic Structure and Spectra (1981)

I.I Sobelman

Atomic Spectra and Radiative Transitions (1979)

A. Thorne et al

Spectrophysics (1999)

L.A. Vainshtein and V.P. Shevelko

Atomic Physics for Hot Plasmas (1993)

H.R. Griem

Plasma Spectroscopy (1964)

Principles of Plasma Spectroscopy (1997)

W. Lochte-Holtgreven (ed.)

Plasma Diagnostics (1968)

D. Salzmann

Atomic Physics in Hot Plasmas (1998)

T. Fujimoto

Plasma Spectroscopy (2004)

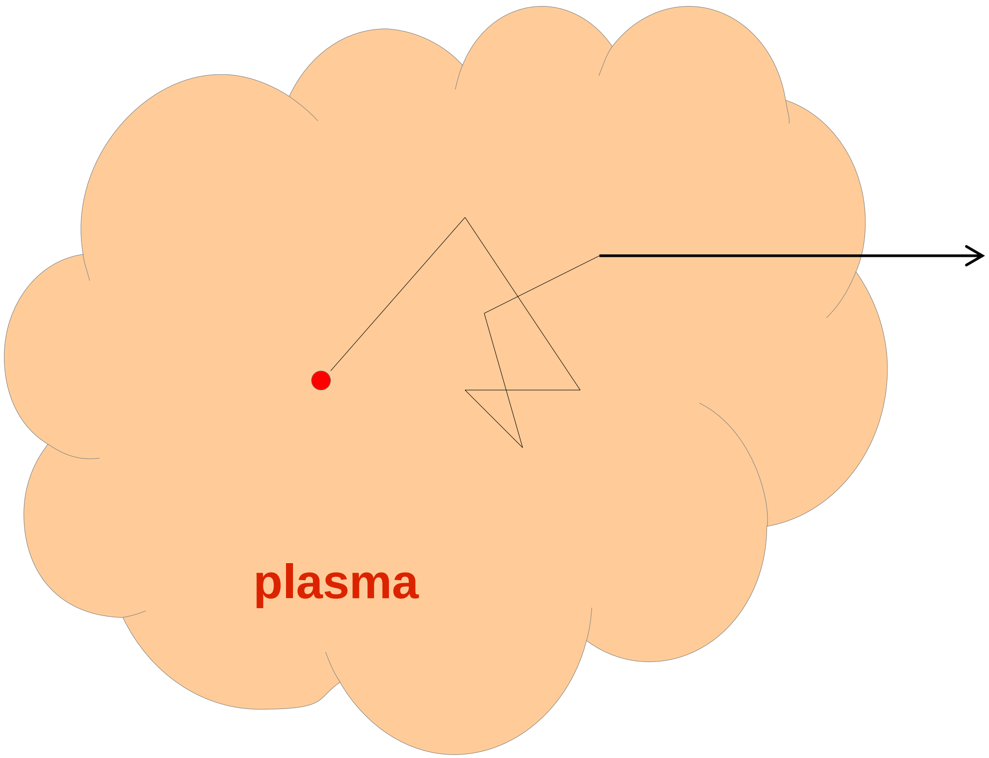
H.-J. Kunze

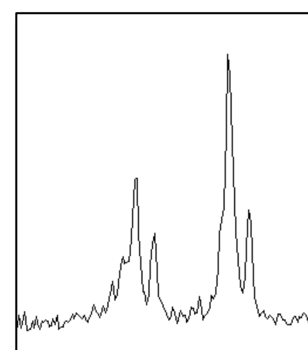
Introduction to Plasma Spectroscopy (2009)

J. Bauche, C. Bauche-Arnoult, O. Peyrusse

Atomic Properties in Hot Plasmas (2015)

Life of a photon





Example: Spectral Line Intensity (thin)

Upper state density (cm^{-3})

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

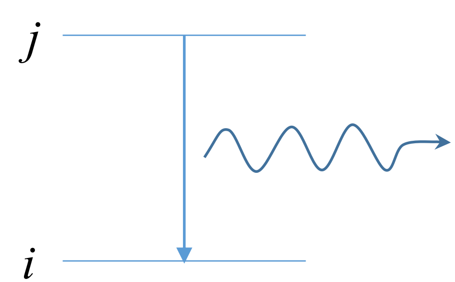
strongly depends on plasma conditions

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

(*almost*) purely atomic parameters

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

Photon energy (eV)



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Types of fundamental atomic data

- Atomic structure
  - Energies, quantum numbers, Lande g-factors
- Radiative
  - Transition wavelengths/energies, transition probabilities (rates), oscillator strengths, lifetimes
- Non-radiative
  - Autoionization rates
- Collisional
  - Cross sections, rate coefficients

Major atomic units/constants

- Energy
  - **1 Ry** ≈ 13.61 eV ≈ 109 737 cm^{-1} = ½ Hartree (a.u.)
    - (*ionization energy of H*)
  - **1 eV** ≈ 8065.5439 cm^{-1}
- Length
  - $\mathbf{a_0}$ ≈ 5.29·10^{-9} cm = 0.529 Å (radius of H atom)
- Area (cross section)
  - $\mathbf{\pi a_0^2}$ ≈ 8.8 ·10^{-17} cm^2 (area of H atom)
- Velocity
  - $\mathbf{v_0}$ ≈ 2.2 ·10^8 cm/s = αc ≈ c/137

- New SI: May 20 2019

https://physics.nist.gov/cuu/Units/

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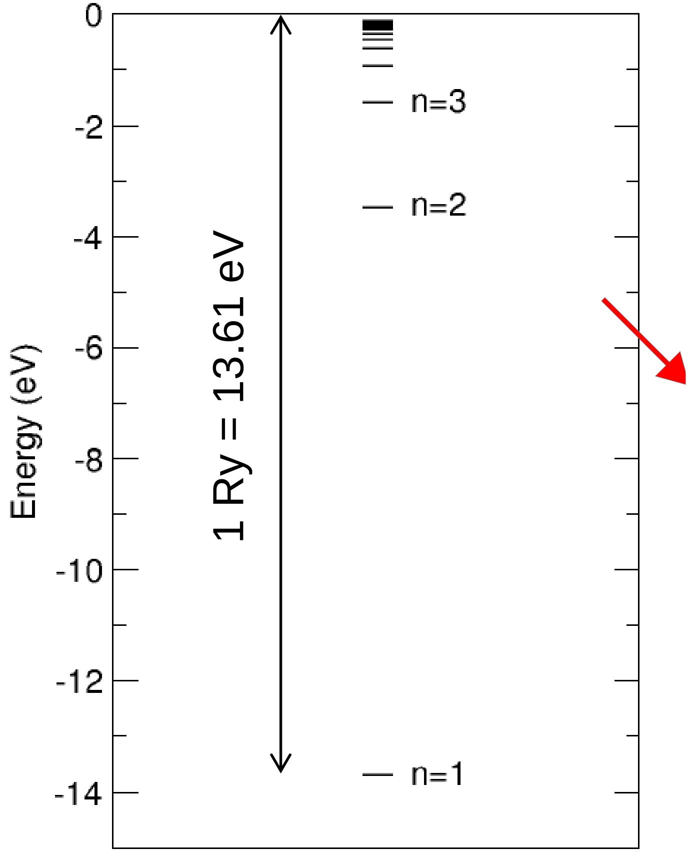
Hydrogen and H-like ions

e.g., E(3s)=E(3p)=E(3d)



Hydrogen atom

H-like Ne?..

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Complex atoms (non-relativistic)

We know all important interactions:

$$H = H_{kin} + H_{elec-nucl} + H_{elec-elec} + H_{s-o} + \ldots$$

$$= -\sum_i \frac{1}{2}\nabla_i^2 - \sum_i \frac{Z}{r_i} + \sum_{i>j} \frac{1}{r_{ij}} + \sum_i \frac{1}{2}\xi_i(r_i)(\boldsymbol{l}_i \cdot \boldsymbol{s}_i) + \ldots$$

$$H\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots) = E\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots)$$

The Schrödinger equation for multi-electron atoms cannot be solved exactly…

“Standard” procedure

- Use central-field approximation to approximate the effects of the Coulomb repulsion among the electrons:
  - $H \approx H_0 = \sum_i^N \left(-\frac{1}{2}\nabla_i^2 \ -\frac{Z}{r_i} + V(r_i) \right)$
- Properly choose the potential V(r)
- Find configuration state functions $\Phi\left(\gamma_j LS\right)$ (accounting also for antisymmetry): ***n***,***l***
- Assume that the atomic state function is a linear combination of CSFs: $\Psi(\gamma LS) = \sum_j^M c_j \Phi\left(\gamma_j LS\right)$
- Solve Schrodinger equation for mixing coefficients:
  - $\left(\hat{H} - E\hat{I}\right)\hat{c} = 0, H_{ij} = \left\langle \Phi(\gamma_i LS) \middle| H \middle| \Phi\left(\gamma_j LS\right) \right\rangle$
- Include other effects (perturbation theory)

Each atomic state (wavefunction) is characterized by a set of quantum numbers

- Generally speaking, **only two are exact**:
  - Total angular momentum (*rotation invariance*)
  - Parity = $(-1)^{\sum_i l_i}$ (*reflection invariance*)

- **Everything else (L,S,*n*,…) is not exact!**

Relativistic atomic structure: heavy and not so heavy ions

$$H_{DC} = \sum_i (c\,\boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + V_{nuc}(r_i) + \beta_i c^2) + \sum_{i>j} \frac{1}{r_{ij}}$$

Dirac-Coulomb Hamiltonian

$\boldsymbol{p} \equiv -i\boldsymbol{\nabla}$ electron momentum operator

$\boldsymbol{\alpha}, \beta$ 4x4 Dirac matrices

$V_{nuc}(r)$ extended nuclear charge distribution

Transverse photons (magnetic interactions and retardation effects):

$$H_{TP} = -\sum_{j>i} \left[\frac{\alpha_i \cdot \alpha_j \cos(\omega_{ij} r_{ij}/c)}{r_{ij}} + (\boldsymbol{\alpha}_i \cdot \boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_j \cdot \boldsymbol{\nabla}_j) \frac{\cos(\omega_{ij} r_{ij}/c) - 1}{\omega_{ij}^2 r_{ij}/c^2} \right]$$

QED effects: self energy (SE), vacuum polarization (VP)

$$H_{DCB+QED} = H_{DC} + H_{TP} + H_{SE} + H_{VP} + \ldots$$

Relativistic notations: one electron

$$\vec{j} = \vec{l} + \vec{s} \qquad j = l \pm 1/2$$

	$s_{1/2}$	$p_{1/2}$	$p_{3/2}$	$d_{3/2}$	$d_{5/2}$	$f_{5/2}$	$f_{7/2}$
	s	p_-	p_+	d_-	d_+	f_-	f_+
l	0	1	1	2	2	3	3
j	½	½	3/2	3/2	5/2	5/2	7/2

Atomic Structure Methods and Codes

- Coulomb approximation (Bates-Damgaard)
- Thomas-Fermi (**SUPERSTRUCTURE**, **AUTOSTRUCTURE**)
- Single-configuration Hartree-Fock (self-consistent field)
  - **Cowan's code + modifications**
- Model potential (including relativistic)
  - **HULLAC**, **FAC**
- Multiconfiguration HF (**`http://nlte.nist.gov/MCHF`**)
- Multiconfiguration Dirac-Hartree-Fock (**MCDHF**)
  - **GRASP2K** (**`http://nlte.nist.gov/MCHF`**)
  - **Desclaux's code**
- Various perturbation theory methods (RMBPT…)
- B-splines

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

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

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

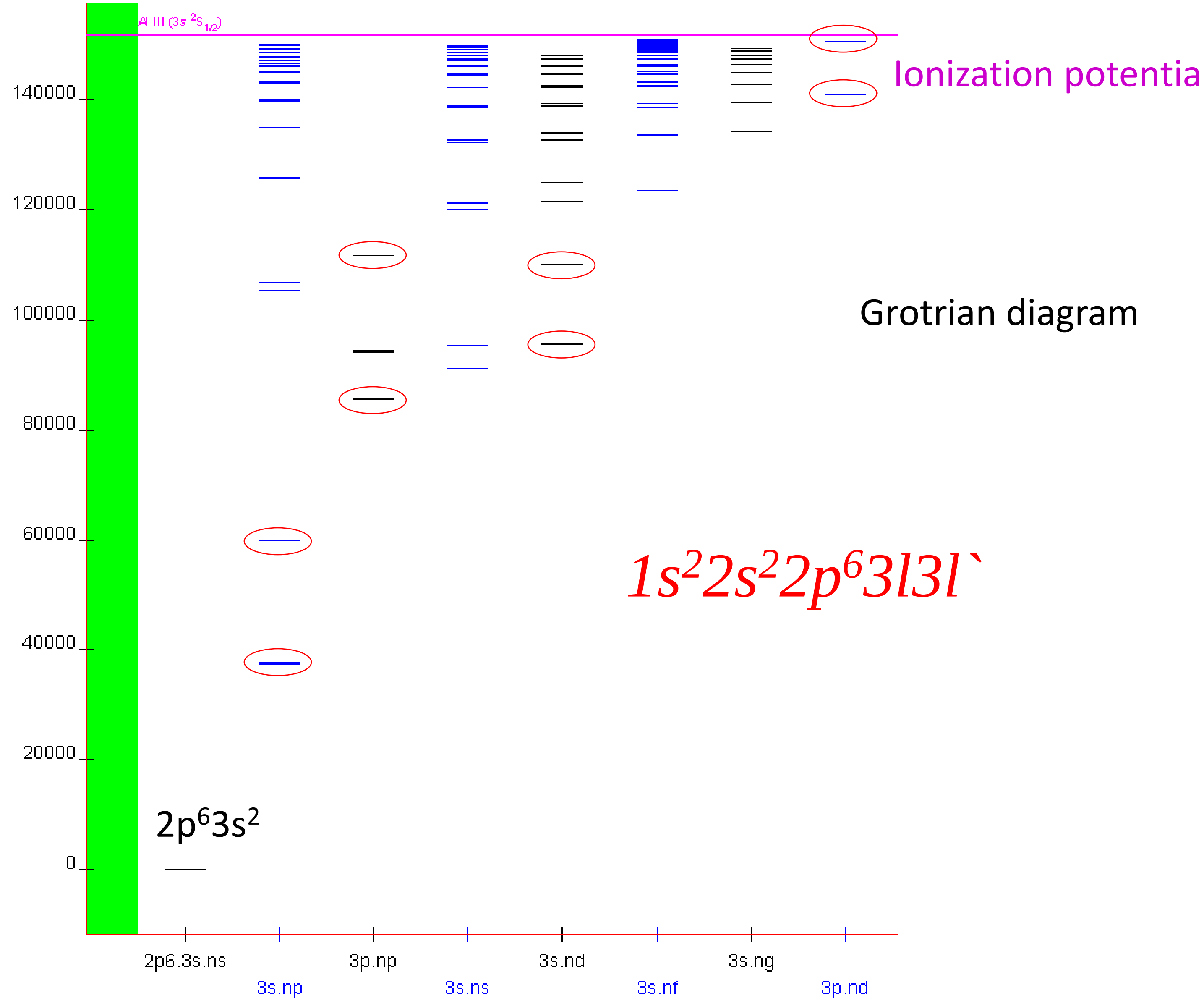
hydrogenic term

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

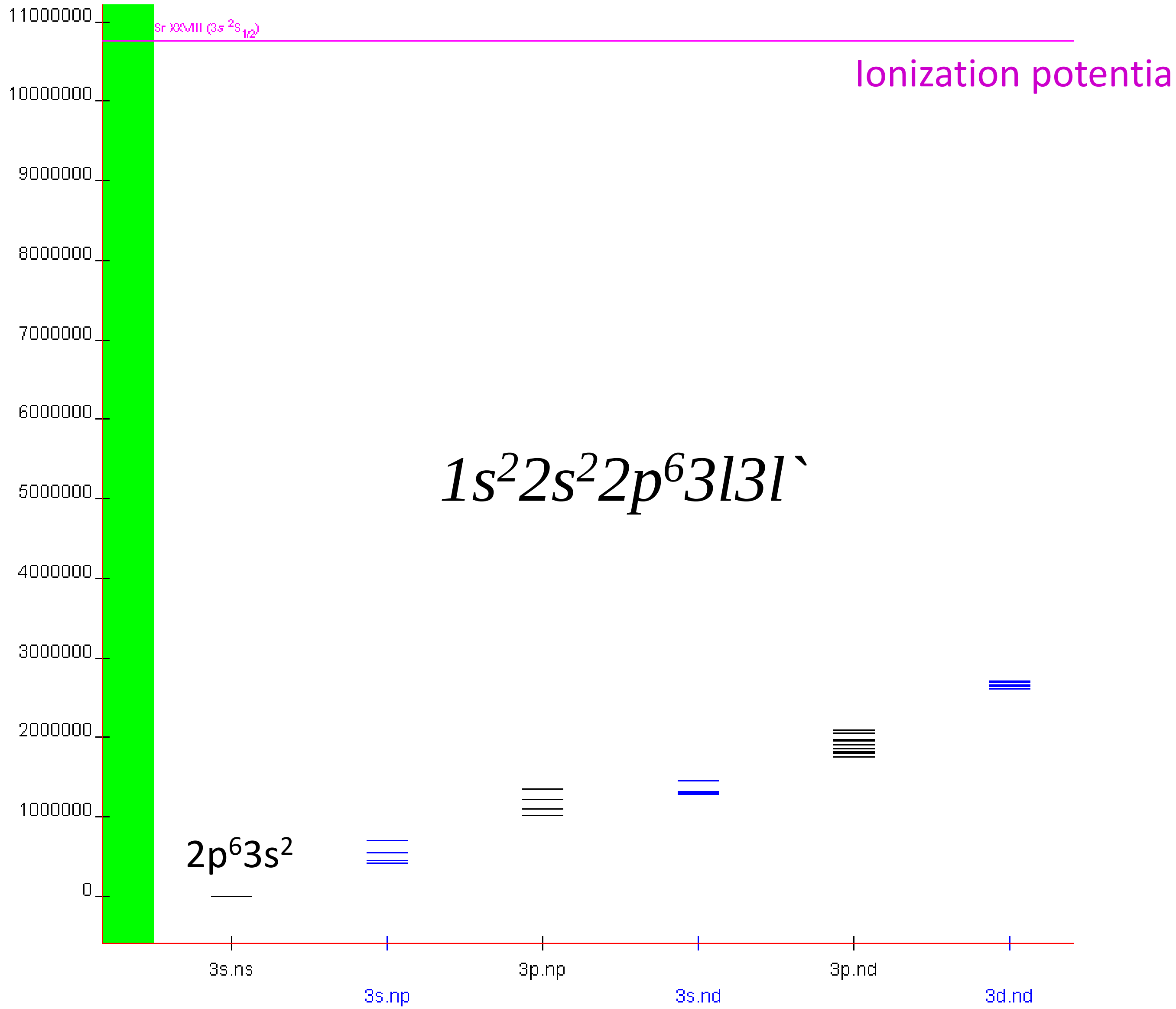
Of course, relativistic effects slightly modify this dependence but the general trend remains valid

IMPORTANT: analysis of **isoelectronic** sequences

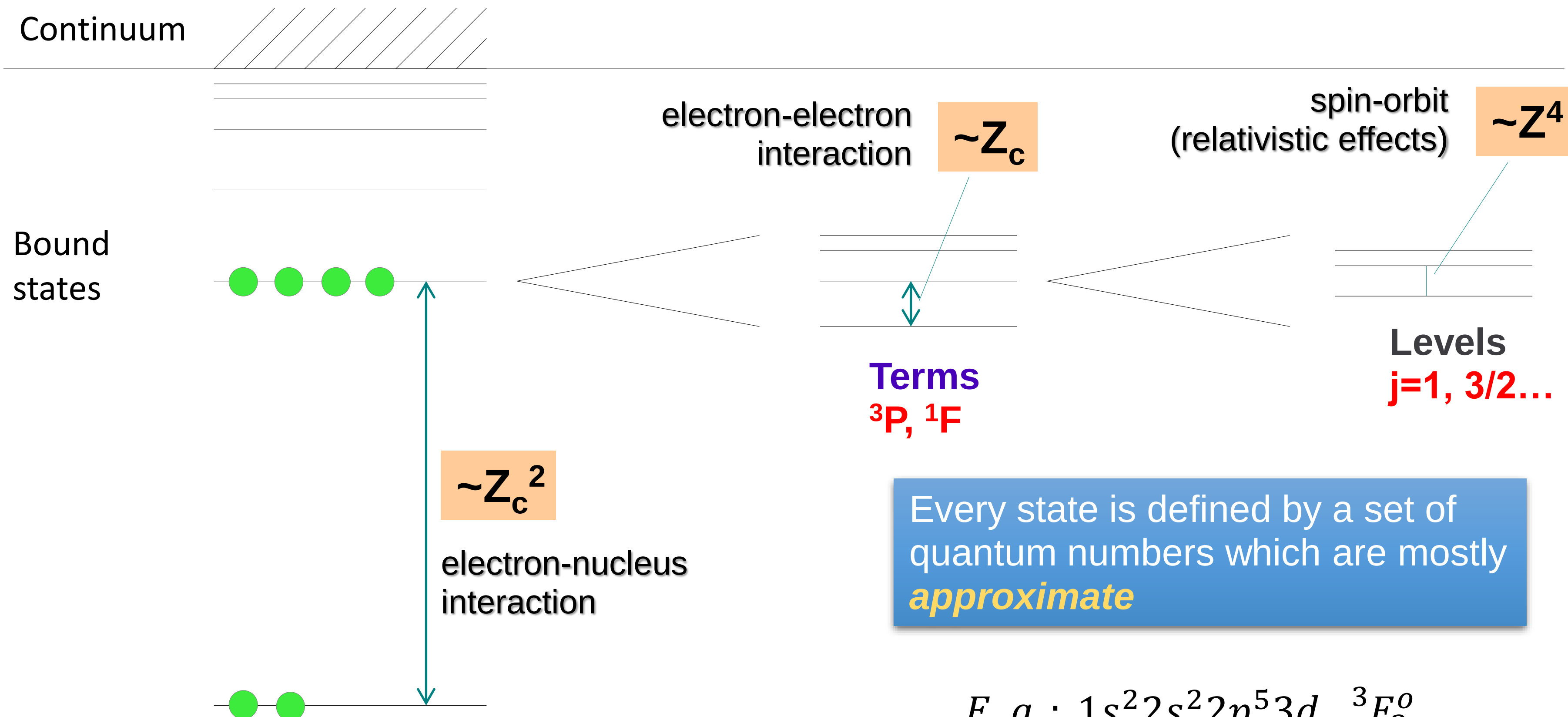
Mg-like Al II: 3l3l'



Mg-like Sr XXVII: 3l3l'



Energy structure of a (relatively light) ion



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

$$E.g.:\ 1s^2 2s^2 2p^5 3d\ \ {}^3F^o_3$$

Electrons are grouped into shells ***nl***
(K n=1, L n=2, M n=3,...)
producing **configurations**

$$\Delta E(\Delta n \neq 0) \sim {Z_c}^2$$
$$\Delta E(\Delta n = 0) \sim Z_c$$

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Spin-orbit (relativistic!) interaction

Hydrogenic ion:
$$\zeta_{nl} = \frac{Ry\,\alpha^2\,Z^4}{n^3\,l\,(l+1/2)\,(l+1)}$$

Semi-theoretical Lande formula:
$$\zeta_{nl} = \frac{Ry\,\alpha^2\,Z_c^2\tilde{Z}^2}{n^{*3}\,l\,(l+1/2)\,(l+1)}$$

n*: effective n
$$IP = \frac{Ry\,Z_c^2}{n^{*2}}$$
(ionization potential)

$\tilde{Z}$: effective nuclear charge (for penetrating orbits) = ***Z-n*** for *np* orbitals

$$H = -\sum_i \frac{1}{2}\nabla_i^2 - \sum_i \frac{Z}{r_i} + \sum_{i>j} \frac{1}{r_{ij}} + \sum_i \frac{1}{2}\xi_i(r_i)(\boldsymbol{l_i}\cdot\boldsymbol{s_i}) + \ \ldots$$

Types of coupling

- **LS-coupling**: electron-electron » spin-orbit
  - light elements $\vec{L} = \vec{l}_1 + \vec{l}_2 + \ldots, \quad \vec{S} = \vec{s}_1 + \vec{s}_2 + \ldots, \quad \vec{J} = \vec{L} + \vec{S}$
  - 2p3p
    - $^1S, ^3S, ^1P, ^3P, ^1D, ^3D$
- **jj-coupling**: spin-orbit » electron-electron
  - heavy elements $\vec{j}_1 = \vec{l}_1 + \vec{s}_1, \ \vec{j}_2 = \vec{l}_2 + \vec{s}_2, \ \ldots \quad \vec{J} = \vec{j}_1 + \vec{j}_2 + \ldots$
  - 2s2p: $(2s_{1/2},2p_{1/2})$ or $(2s,2p_-)$
  - $3d^5$: $((3d_-^3)_{5/2},(3d_+^2)_2)_{3/2}$
- ***Intermediate coupling***
  - neither LS or jj is overwhelmingly strong
- Other types of couplings exist (jK, LK, J_1J_2,…)

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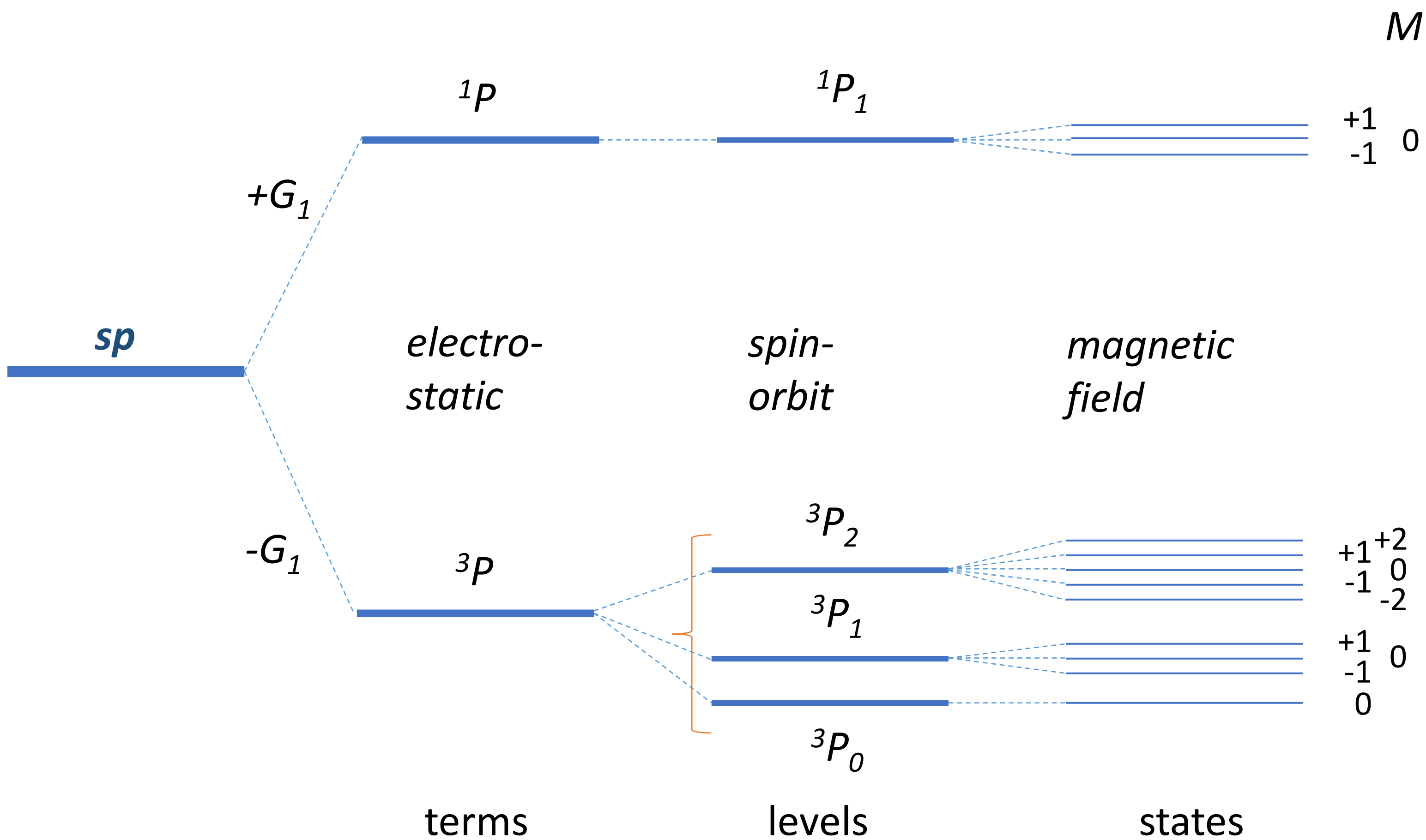
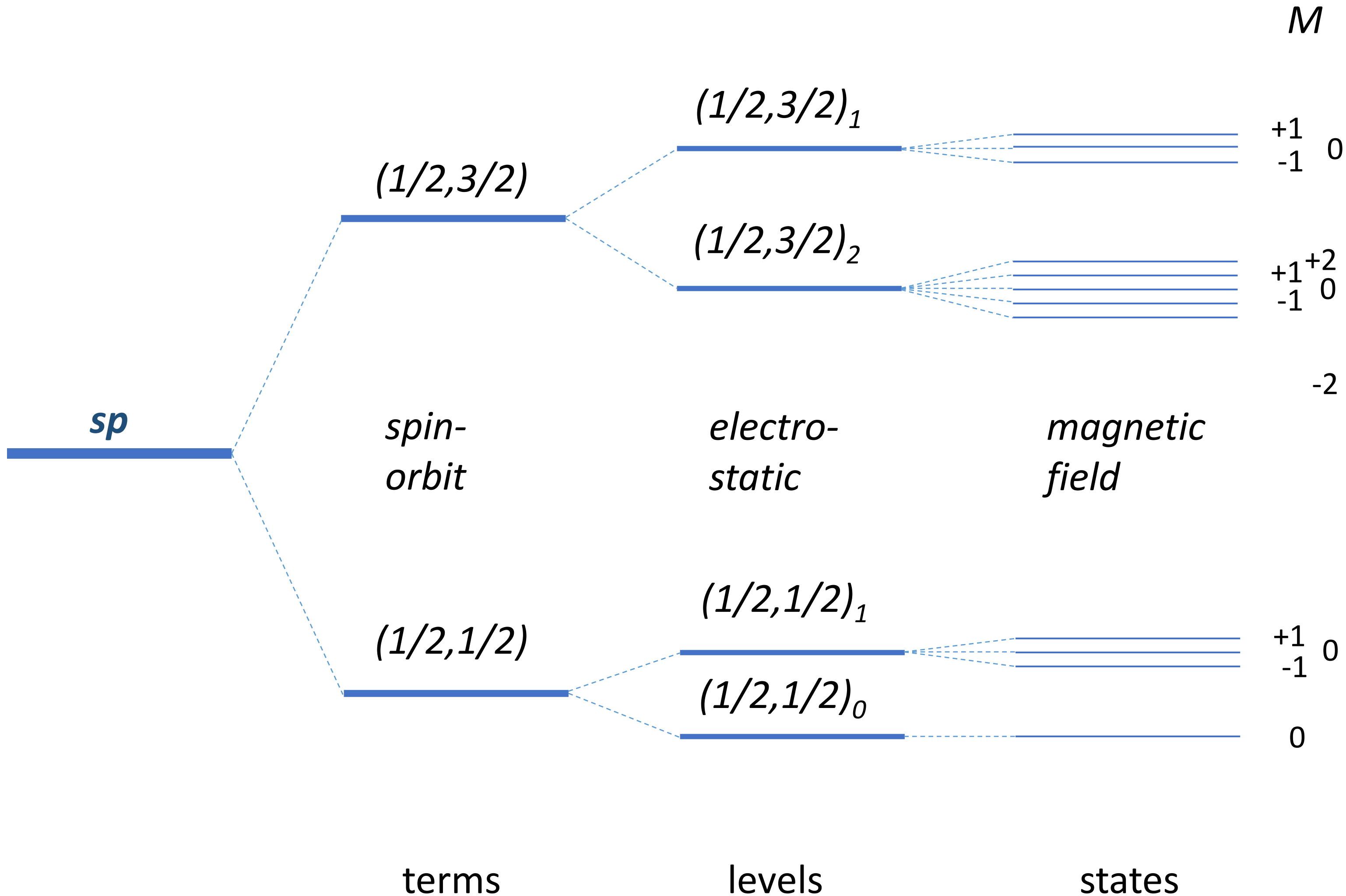
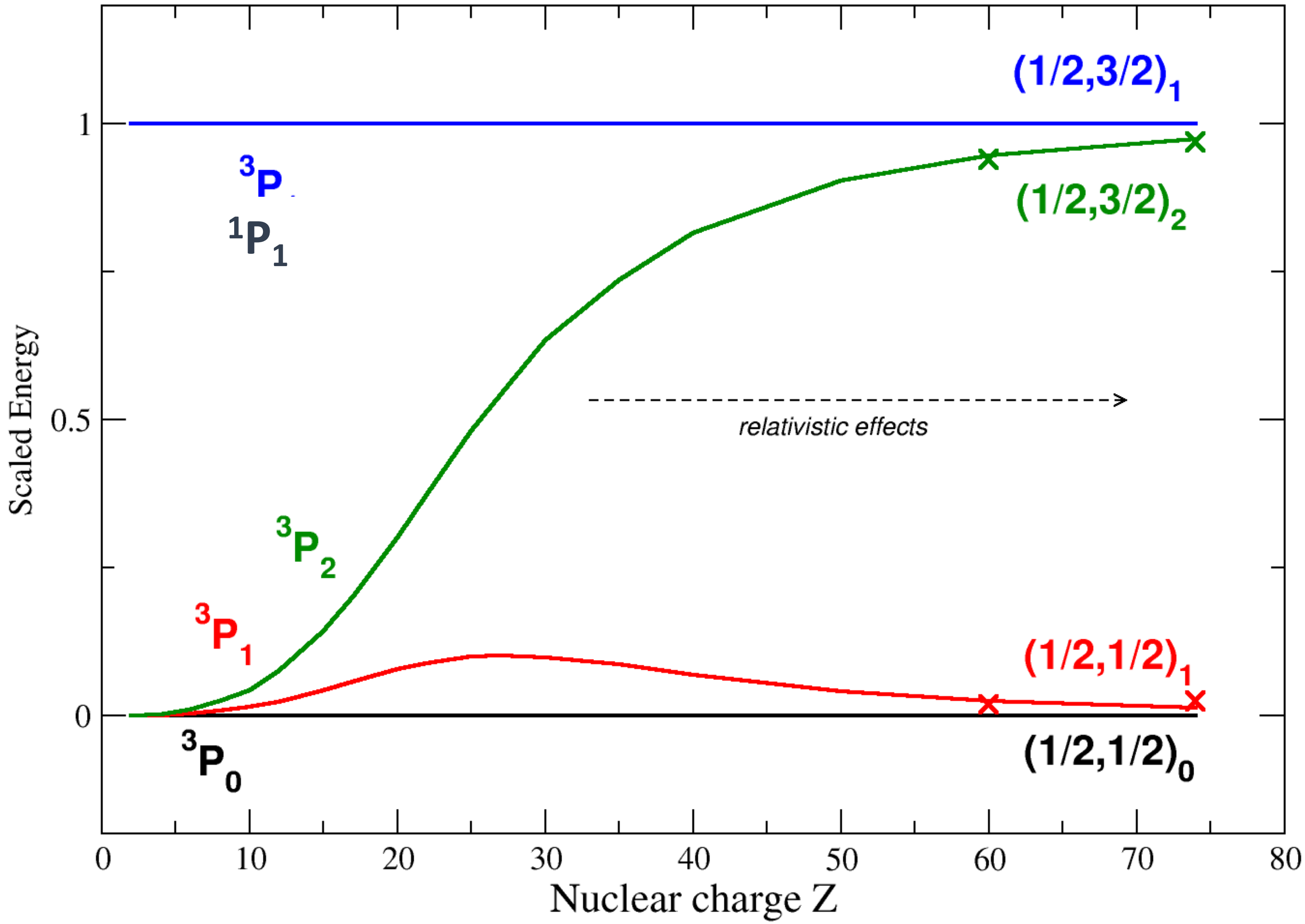
Configuration ***nsn`p***: LS coupling (LSJ)



Configuration ***nsn`p***: jj coupling



From LS to jj: **1*s*2*p*** in He-like ions



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State mixing: intermediate coupling, configuration interaction

$$|\Psi(a,b,c,\ldots)\rangle = \sum_i \alpha_i \Psi_i(a',b',c',\ldots)$$

expansion coefficients

He-like Na^{9+}: $1s2p\ ^3P_1 = \mathbf{0.999}\ ^3P + \mathbf{0.032}\ ^1P$
He-like Fe^{24+}: $1s2p\ ^3P_1 = \mathbf{0.960}\ ^3P + \mathbf{0.281}\ ^1P$
He-like Mo^{40+}: $1s2p\ ^3P_1 = \mathbf{0.874}\ ^3P + \mathbf{0.486}\ ^1P$

s-o coupling increases with Z $\Rightarrow$ change of coupling scheme

Very, VERY important for radiative transitions!!!

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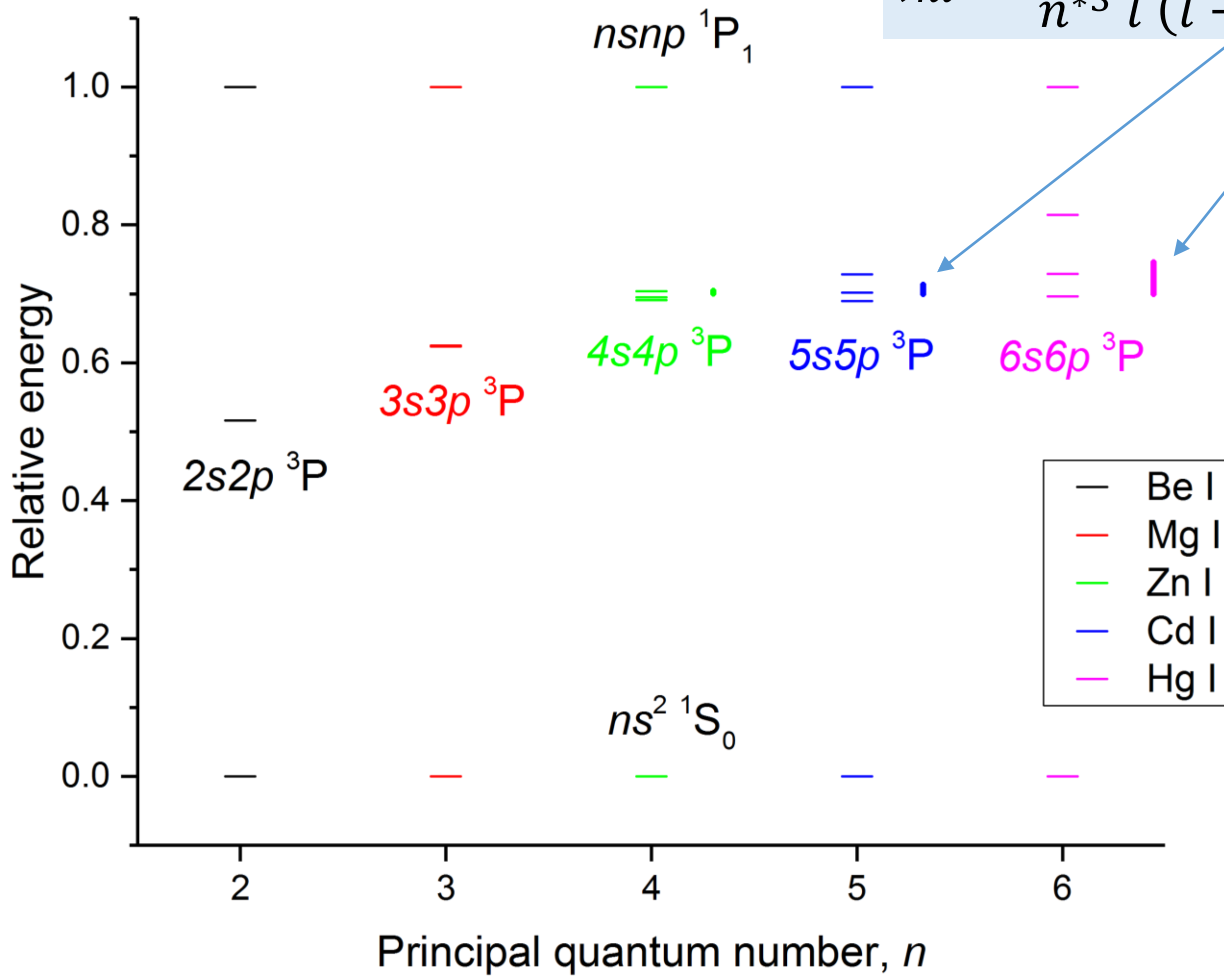
Spin-orbit interaction does depend on nuclear charge!

$$\zeta_{nl} = \frac{Ry\ \alpha^2\ Z_c^2 \tilde{Z}^2}{n^{*3}\ l\,(l+1/2)\,(l+1)}$$

Lande formula



Non-trivial coupling (J_1J_2)

Np-like ion: 93 electrons

Closed shells: unimportant

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 4f^{14} 5s^2 5p^6 5d^{10} 5f^4 6s^2 6p^6 6d 7s 7p$

J=9/2

$5f^4(^5I_4)6d_{3/2}\ \ (4,{}^3/_2)_{11/2} 7s7p(^1P^\circ{}_1)\ \ ({}^{11}/_2, 1)^\circ{}_{\mathbf{9/2}}$

Non-trivial coupling (J_1J_2)

Np-like ion: 93 electrons

Closed shells: unimportant

$1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}4f^{14}5s^25p^65d^{10}5f^46s^26p^66d7s7p$

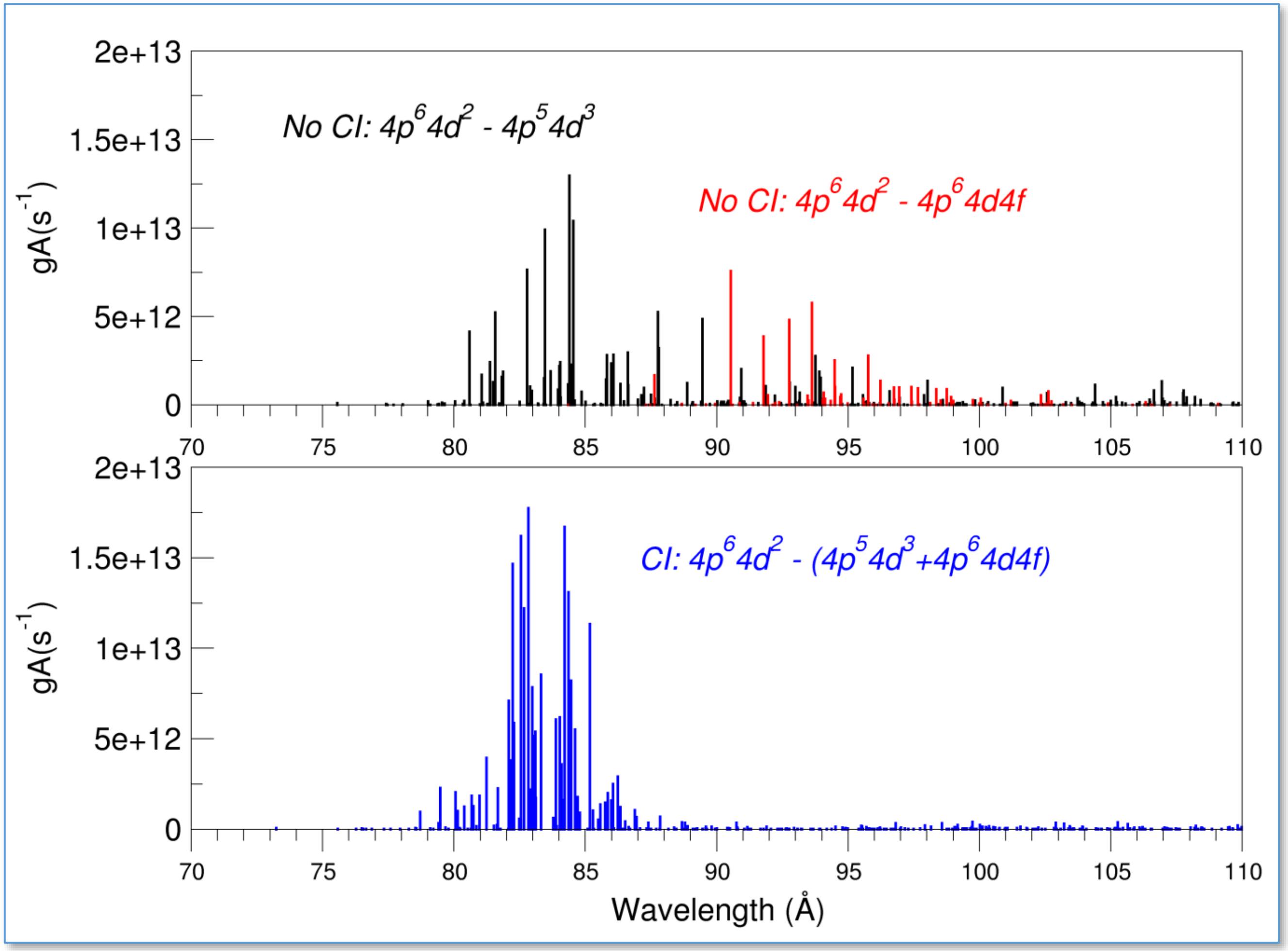
J=9/2

$5f^4(^5I_4)6d_{3/2}\ (4,{}^3/_2)_{11/2}7s7p(^1P^\circ_1)\ ({}^{11}/_2,\ 1)^\circ_{9/2}$

Configuration interaction example

From J. Bauche et al

Pr XXII: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^2$



Hund's rules (equivalent electrons, LS)

- Largest S has the lowest energy
- Largest L with the same S has the lowest energy
- For atoms with less-than half-filled shells, lowest J has lowest energy

- Lande interval rule:
  - $E(J)-E(J-1) = \beta J$

C I

Configuration	Term	J	Level (cm^{-1})	Reference
$2s^22p^2$	^3P	0	0.00	L7288
		1	16.40	
		2	43.40	
$2s^22p^2$	^1D	2	10 192.63	
$2s^22p^2$	^1S	0	21 648.01	
$2s2p^3$	$^5S°$	2	33 735.20	
$2s^22p3s$	$^3P°$	0	60 333.43	
		1	60 352.63	
		2	60 393.14	
$2s^22p3s$	$^1P°$	1	61 981.82	
$2s2p^3$	$^3D°$	3	64 086.92	
		1	64 089.85	
		2	64 090.95	

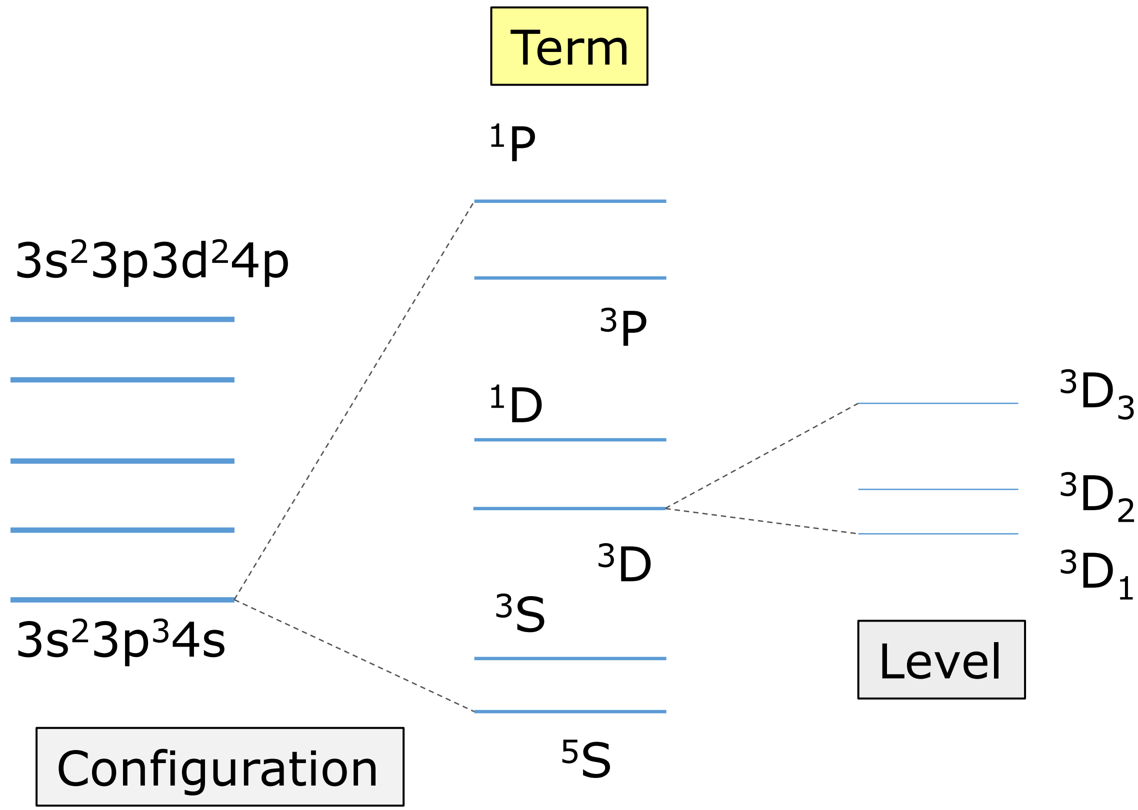
S I

- For atoms with more-than half-filled shells, largest *J* has lowest energy

- Lande interval rule:
  - $E(J)-E(J-1) = \beta J$

Configuration	Term	*J*	Level (cm^{-1})
$3s^23p^4$	^3P	2	0.000
		1	396.055
		0	573.640
$3s^23p^4$	^1D	2	9 238.609
$3s^23p^4$	^1S	0	22 179.954
$3s^23p^3(^4S^\circ)4s$	$^5S^\circ$	2	*52 623.640*
$3s^23p^3(^4S^\circ)4s$	$^3S^\circ$	1	*55 330.811*
$3s^23p^3(^4S^\circ)4p$	^5P	1	63 446.065
		2	63 457.142
		3	63 475.051

16-electron ion (S-like)



Even parabolic states for motional Stark effect!

Superconfigurations

Motivation: for very complex atoms (ions) not only the **number of levels** is overwhelmingly large, but also the **number of configurations**

Example:

$1s^2 2s^2 2p^5 3s$
$1s^2 2s^2 2p^5 3p$
$1s^2 2s^2 2p^5 3d$
$1s^2 2s 2p^6 3s$
$1s^2 2s 2p^6 3p$
$1s^2 2s 2p^6 3d$

→

different *n*'s

$(1s)^2(2s2p)^7(3s3p3d)^1 \equiv (1)^2(2)^7(3)^1$

BUT: $(1s)^2(2s2p)^7(3s3p3d4s4p4d4f)^1$

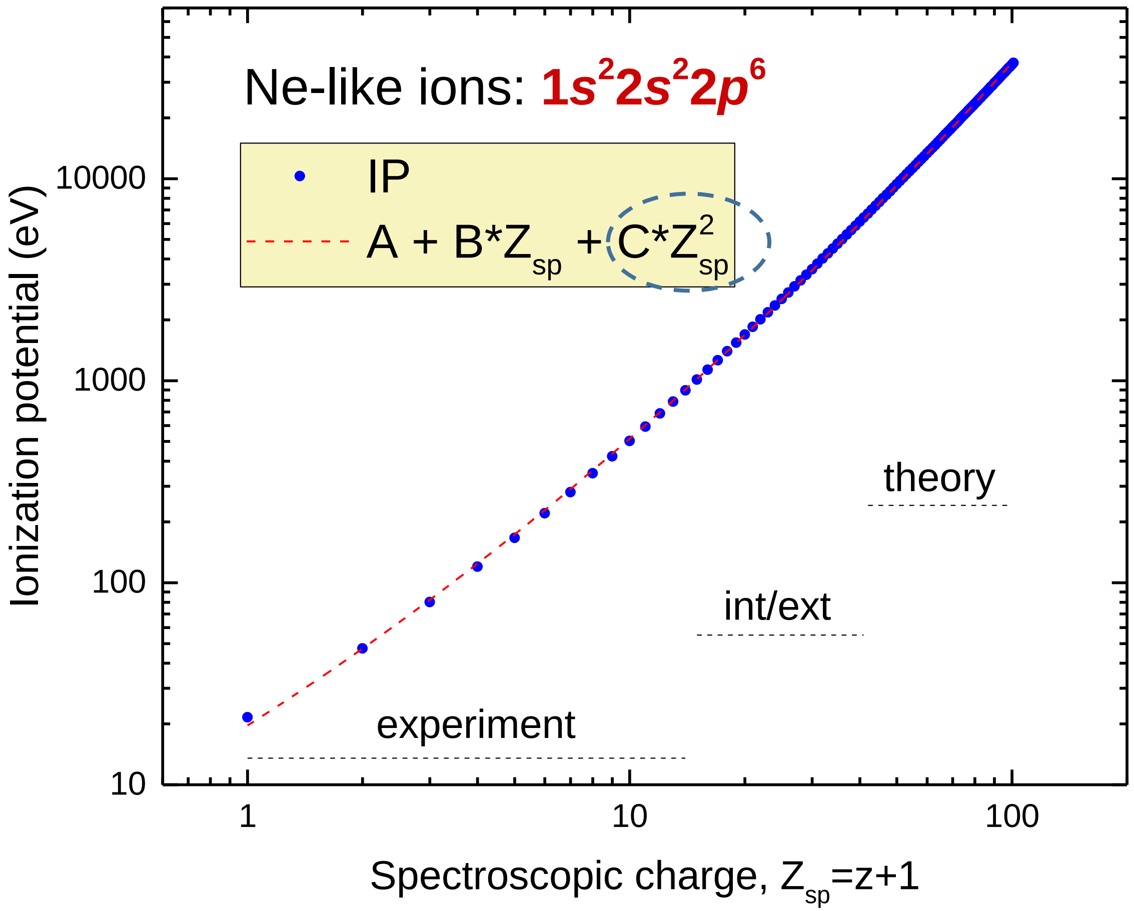
Instead of producing millions or billions of lines, SCs are used to calculate Super Transition Arrays → Statistical methods

FLYCHK, CRETIN, DEDALE…

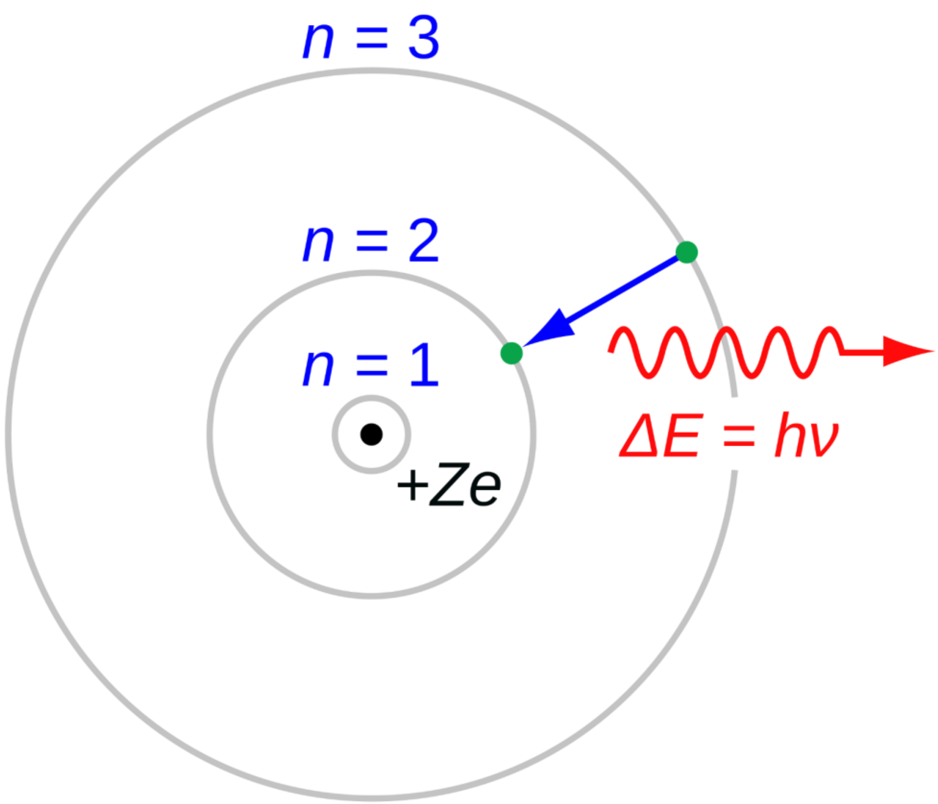
See J. Bauche et al's book (2015)

Ionization potentials

- IPs are directly connected with ionization distributions in plasmas
- Most often are determined from Rydberg series

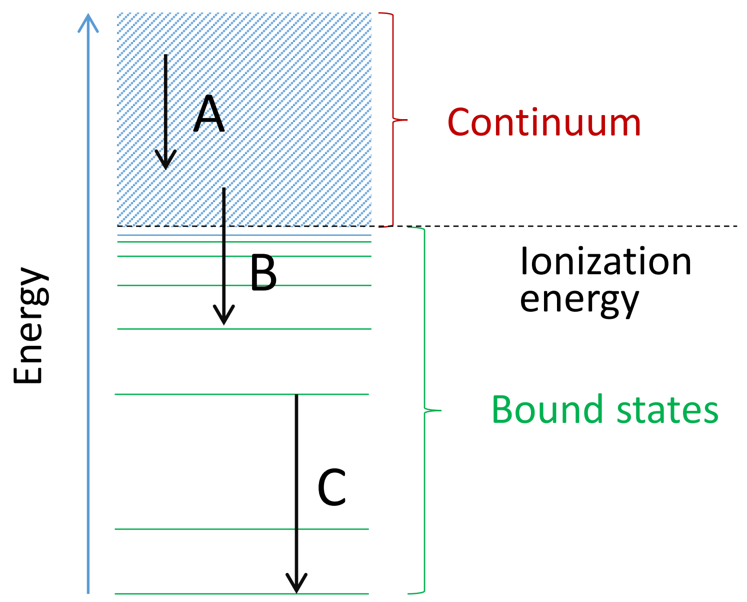


Now to radiative processes…



Three major sources of photons

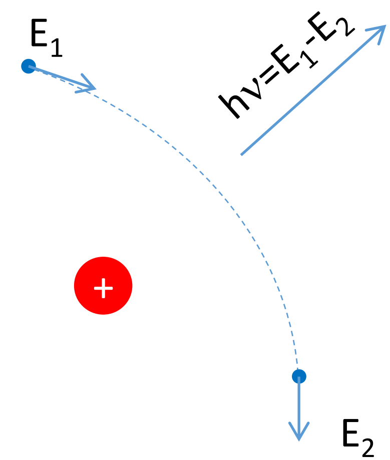
- Free-free transitions (bremsstrahlung)
  - $A^{z+} + e \rightarrow A^{z+} + e + h\nu$
- Free-bound transitions (radiative recombination)
  - $A^{z+} + e \rightarrow A^{(z-1)+} + h\nu$
- Bound-bound transitions
  - $A_j^{z+} \rightarrow A_i^{z+} + h\nu$



•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 $\lambda \frac{620\ nm}{T_e[eV]}_{\max}$

Atomic Processes

Almost all relevant physics is inside this matrix element

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

final state

interaction operator

initial state

- Wavelengths
- Energies
- Transition probabilities (radiative and non-radiative)
- Collisional cross sections
- …

Radiative transitions: decay rate

- Classical rate of loss of energy: dE/dt ~ |**a**|^2, and decay rate ~ |**r**|^2 for harmonic oscillator

- Quantum treatment:

$$\left\langle \Psi_f \middle| \vec{\varepsilon} \cdot \vec{p}\; e^{i\vec{k}\vec{r}} \middle| \Psi_i \right\rangle$$

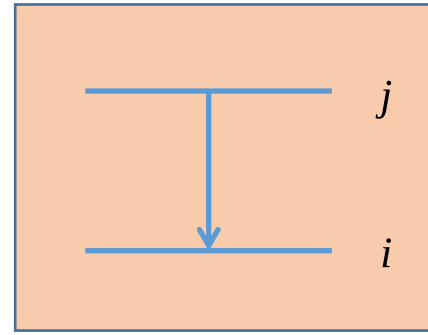
  - e^{ikr} = 1+***ikr***+… ≈ 1 (electric dipole or E1 – allowed)
  - Velocity form:
  - Length form:

$$\langle \Psi_f | \nabla | \Psi_i \rangle$$

$$\langle \Psi_f | r | \Psi_i \rangle$$

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

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*)

  $$f_{ji} = \frac{1}{3g_i}\frac{\Delta E}{Ry}S$$

  - $g_j f_{ij} = g_i f_{ji}$ ($g_j = 2J_j+1$);   dimensionless
  - Typical values for strong lines: ~ 0.1-1

- **Transition probability** (or Einstein coefficient)

$$A_{ij}[s^{-1}] = 4.34 \cdot 10^7 \frac{g_i}{g_j}(\Delta E[eV])^2 f_{ji}$$

- Typical values for neutrals: $\sim 10^8$ s^{-1}

Selection rules and Z-scaling

Fundamental law:
parity and J do not change

Before:	P_j	$\vec{J}_j$
After:	$P_i \cdot P_{ph}$	$\vec{J}_i + \vec{J}_{ph}$

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

Exact selection rules:
$P_j = - P_i$
$|\Delta J| \leq 1,\ 0 \nrightarrow 0\ (J_j+J_i \geq 1)$

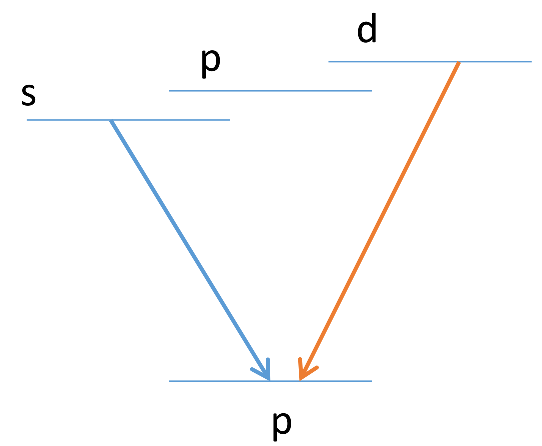
Approximate selection rules (for LS coupling):
$\Delta S = 0,\ |\Delta L| \leq 1,\ 0 \nrightarrow 0$

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

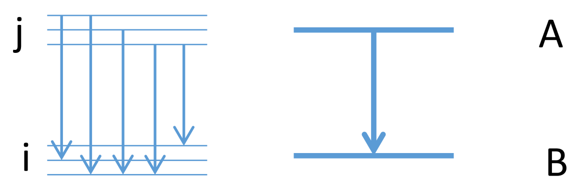
- **$\Delta n \neq 0$**
  - $r \propto Z^{-1} \Rightarrow$ **$S \propto Z^{-2}$**
  - $\Delta E \propto Z^2 \Rightarrow$ **$f \propto Z^0$**
  - **$A \propto Z^4$**
- **$\Delta n = 0$**
  - $r \propto Z^{-1} \Rightarrow$ **$S \propto Z^{-2}$**
  - $\Delta E \propto Z \Rightarrow$ **$f \propto Z^{-1}$**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

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



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

Level => term => configuration => …

Principal quantum number *n*

- *n*-dependence for *f*:

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

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

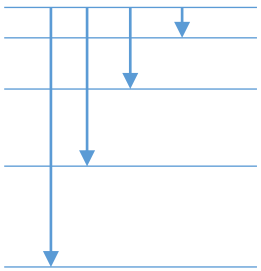
$$f(n_2 >> n_1) \propto \frac{1}{\boldsymbol{n}_2^3}$$

- *n*-dependence for *A*

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

- Total radiative rate from a specific *n*

$$A_Z(n) \approx 1.6 \times 10^{10}\,\frac{\boldsymbol{Z}^4}{n^{9/2}}\,(s^{-1})$$



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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
  - $\boldsymbol{A} \propto \boldsymbol{Z}^6$ or stronger
  - Same parity, $|\Delta J| \leq 1$, $J_j + J_i \geq 1$
- Electric quadrupole (E2)
  - Stronger between configurations/terms
  - $\boldsymbol{A} \propto \boldsymbol{Z}^6$ or stronger
  - Same parity, $|\Delta J| \leq 2$, $J_j + J_i \geq 2$

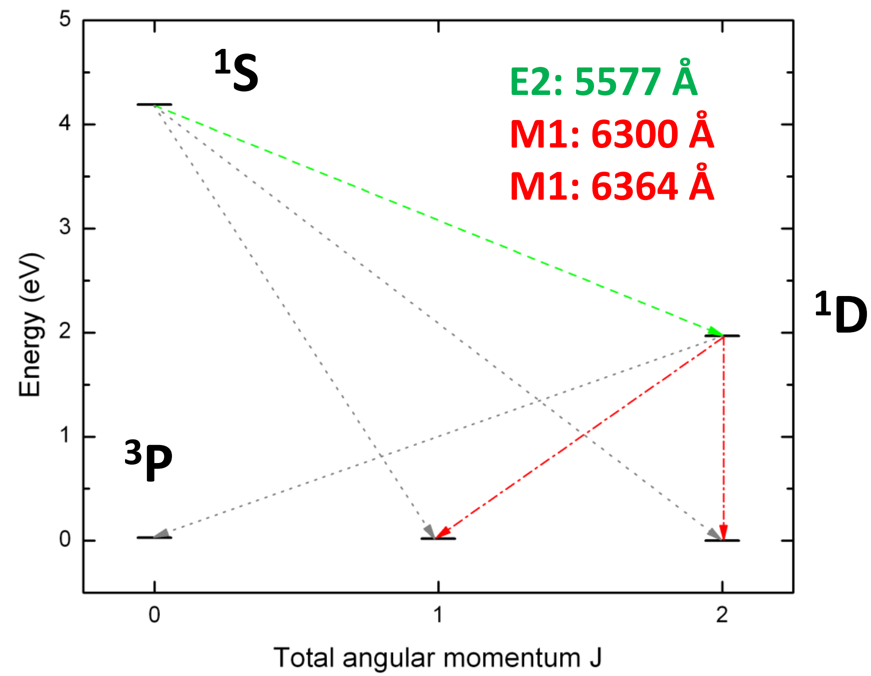
Generally weak…

Aurora borealis

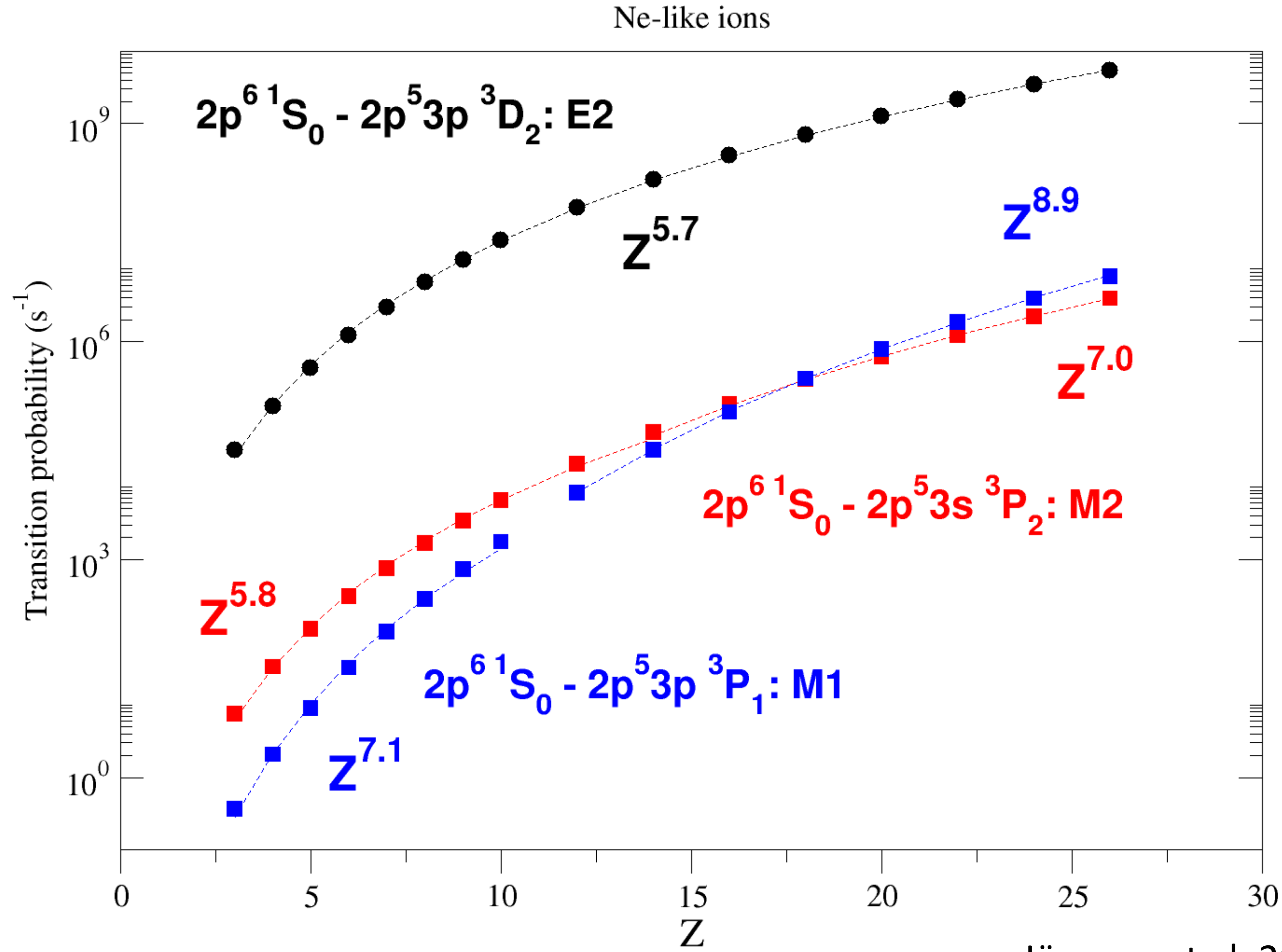
Forbidden transitions: auroras

O I $2p^4$

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)



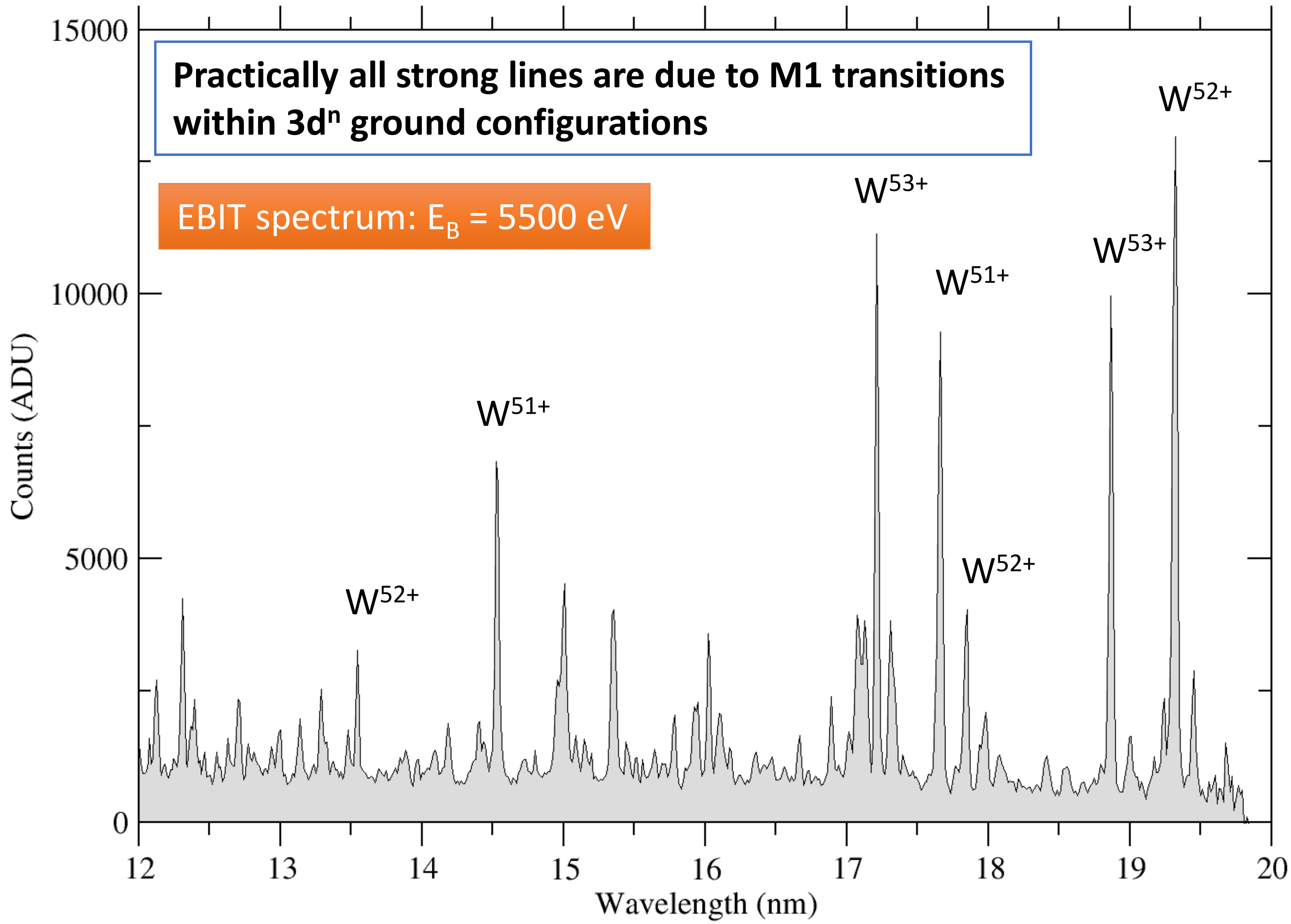
Scaling in Ne-like ions



Jönsson et al, 2011

Forbidden transitions: highly-charged W

$A \sim 10^4$-10^6 s^{-1}



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Relativistic atomic structure: heavy and not so heavy ions

$$H_{DC} = \sum_i (c\,\boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + V_{nuc}(r_i) + \beta_i c^2) + \sum_{i>j} \frac{1}{r_{ij}}$$

Dirac-Coulomb Hamiltonian

$\boldsymbol{p} \equiv -i\boldsymbol{\nabla}$ electron momentum operator

$\boldsymbol{\alpha}, \beta$ 4x4 Dirac matrices

$V_{nuc}(r)$ extended nuclear charge distribution

Transverse photons (magnetic interactions and retardation effects):

$$H_{TP} = -\sum_{j>i} \left[\frac{\alpha_i \cdot \alpha_j \cos(\omega_{ij} r_{ij}/c)}{r_{ij}} + (\boldsymbol{\alpha}_i \cdot \boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_j \cdot \boldsymbol{\nabla}_j) \frac{\cos(\omega_{ij} r_{ij}/c) - 1}{\omega_{ij}^2 r_{ij}/c^2} \right]$$

QED effects: self energy (SE), vacuum polarization (VP)

$$H_{DCB+QED} = H_{DC} + H_{TP} + H_{SE} + H_{VP} + \ldots$$

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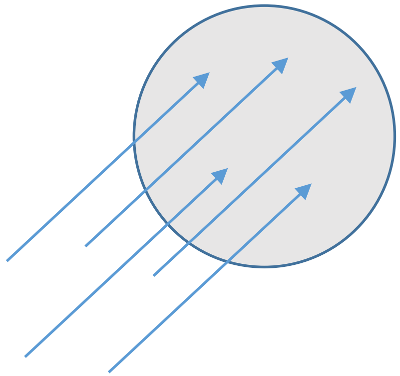
Collisions in plasmas

- More than one particle: collisions!
- Elastic, inelastic



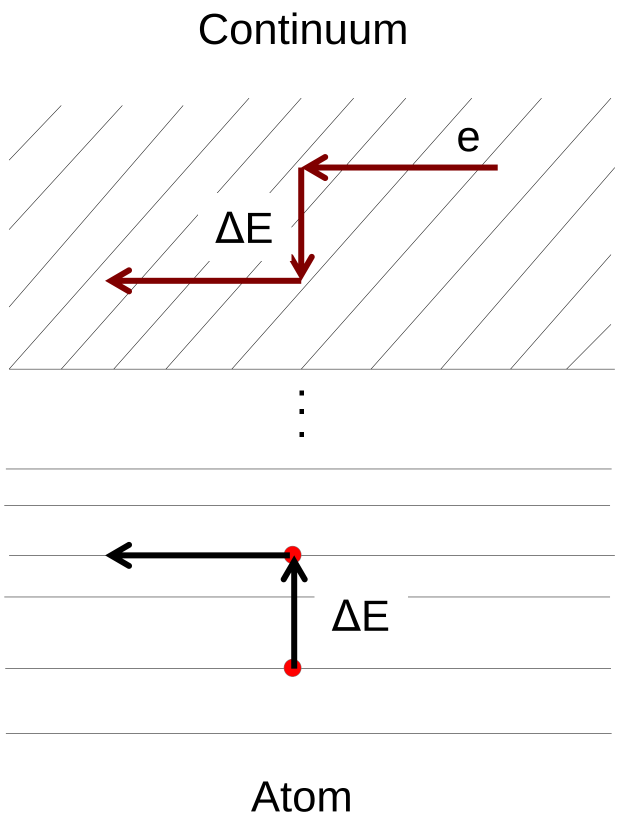
Number of collisions per unit time:

n[1/cm^3]*v[cm/s]*Area[cm^2] ~ [1/s]

Equilibrium plasma: $T_e = T_A$

$$\frac{v_e}{v_A} = \sqrt{\frac{M}{m_e}}$$

Collision (excitation)



Main *binary* quantity: cross section **σ(E)** **[cm²]**

Effective area for a particular process

$$\sigma(E) = \int |f(E,\theta,\phi)|^2 \, d\Omega$$

f is the scattering amplitude

Process rate in plasmas:

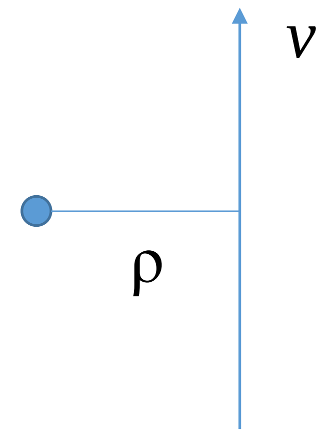
$$R[s^{-1}] = n\langle\sigma \mathrm{v}\rangle \equiv n \int_{E_{\min}}^{E_{\max}} \sigma(E)\cdot \mathrm{v}(E)\cdot f(E)dE$$

rate coefficient

Basic Parameters

- Cross sections are probabilities
  - Classically:

$$\sigma(\Delta E, E) = \int_0^\infty P(\Delta E, E, \rho) \cdot 2\pi\rho d\rho$$

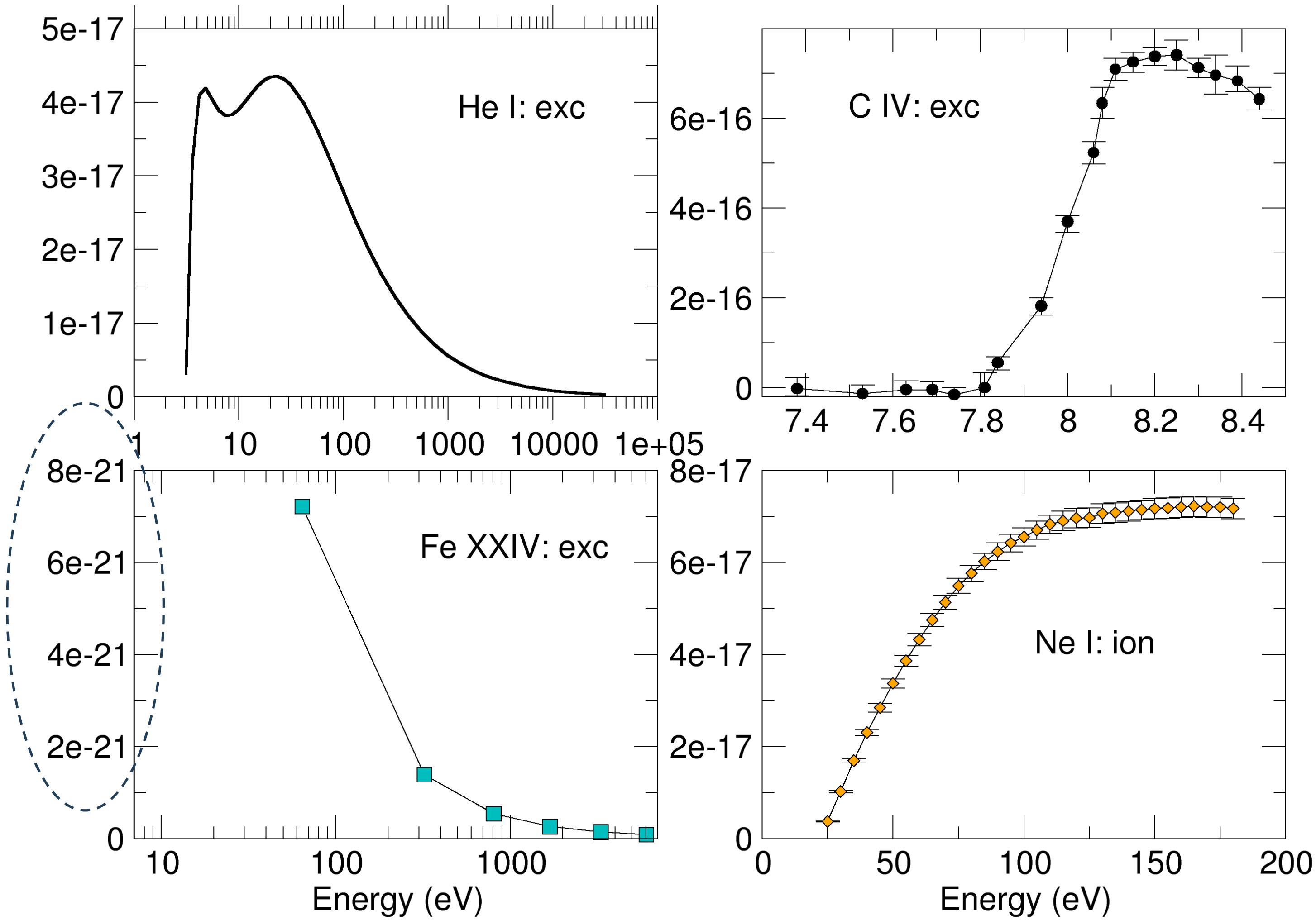


- Typical values for atomic cross sections
  - $a_0 \sim 5{\cdot}10^{-9}$ cm $\Rightarrow \pi a_0^{\,2} \sim \mathbf{10^{-16}\ cm^2}$
- Collision strength Ω (dimensionless, *on the order of unity*):

$$\sigma_{ij}(E) = \pi a_0^2 \frac{Ry}{g_j E} \Omega_{ij}(E)$$

  - Ratio of cross section to the de Broglie wavelength squared
  - Symmetric w/r to initial and final states

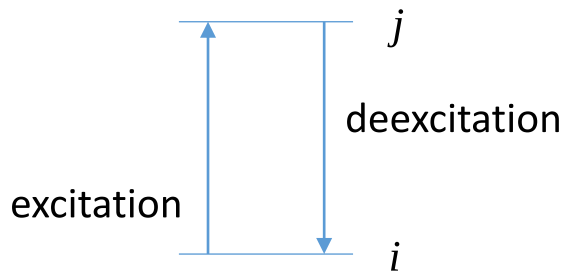
Examples: excitation and ionization (cm^2)



Direct and inverse

- Quantum mechanics tells us that characteristics of direct and inverse processes are related

ΔE is the excitation threshold



$$\Omega_{ij}(E+\Delta E)=\Omega_{ji}(E)$$

Klein-Rosseland formula:

$$g_i(E+\Delta E)\sigma_{exc}(E+\Delta E)=g_j E\sigma_{dxc}(E)$$

$$A(i)+e\leftrightarrow A(j)+e$$

Rates: $g_i\langle\sigma v\rangle_{exc}=g_j\langle\sigma v\rangle_{dxc}\cdot e^{-\Delta E/T}$

Milne formula for photoionization/photorecombination: $\hbar\omega=E+I_Z$

$$A+h\nu\leftrightarrow A^{+}+e$$

$$g_z\sigma_{ph}(\hbar\omega)=\frac{2mc^2}{\hbar^2\omega^2}g_{z+1}\sigma_{rr}(E)$$

Types of transitions for excitation

Examples in He I:

- Optically(dipole)-allowed
  - $P \cdot P' = -1$ (different parity)
  - $|\Delta l| = 1$
  - $\Delta S = 0$
  - $\sigma(E \to \infty) \sim \ln(E)/E$

$1s^2\ {}^1S \to 1s2p\ {}^1P$
$1s2p\ {}^3P \to 1s4d\ {}^3D$

- Optically(dipole)-forbidden
  - $\Delta S = 0$
  - $\sigma(E \to \infty) \sim 1/E$

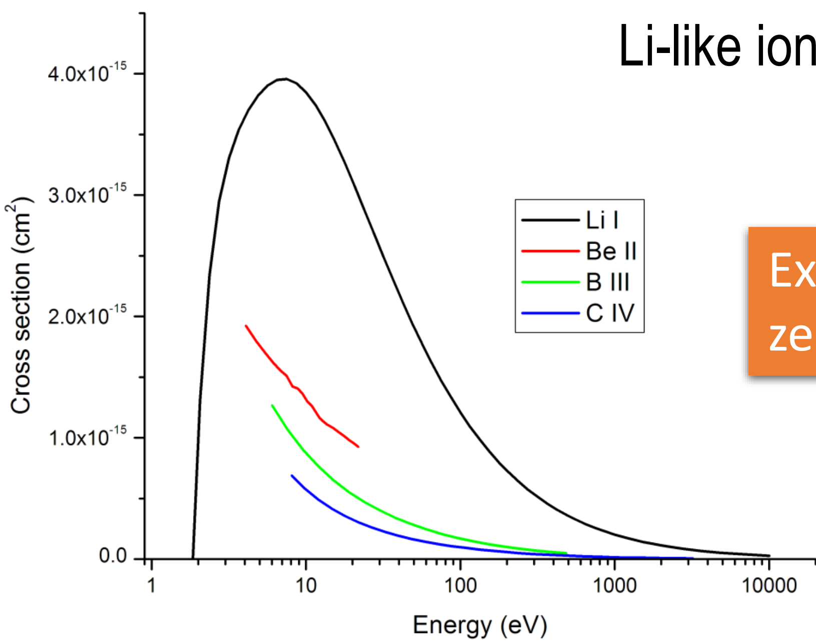
$1s2s\ {}^1S \to 1s3s\ {}^1S$
$1s2s\ {}^3S \to 1s4d\ {}^3D$

- Spin-forbidden (EXCHANGE!)
  - $\Delta S \neq 0$
  - $\sigma(E \to \infty) \sim 1/E^3$

$1s^2\ {}^1S \to 1s2p\ {}^3P$
$1s2p\ {}^3P \to 1s4d\ {}^1D$

Order of cross sections

- *General* order
  - *optically allowed > optically forbidden > spin forbidden*
- OA: long-distance, similar to E1 radiative transitions
- The larger Δl, the smaller cross section



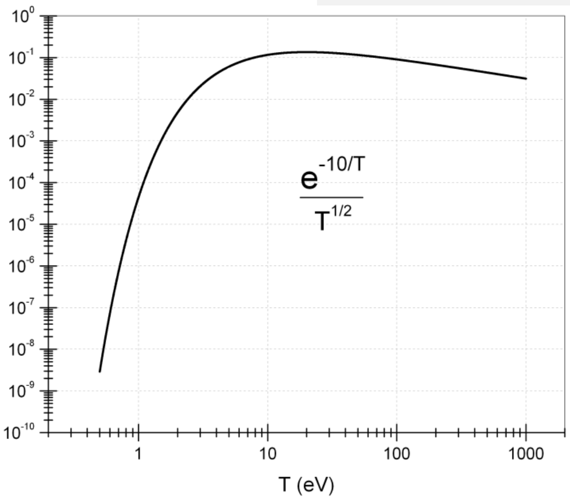
Excitation cross sections for ions are **NOT** zero at the threshold

From cross sections to rates

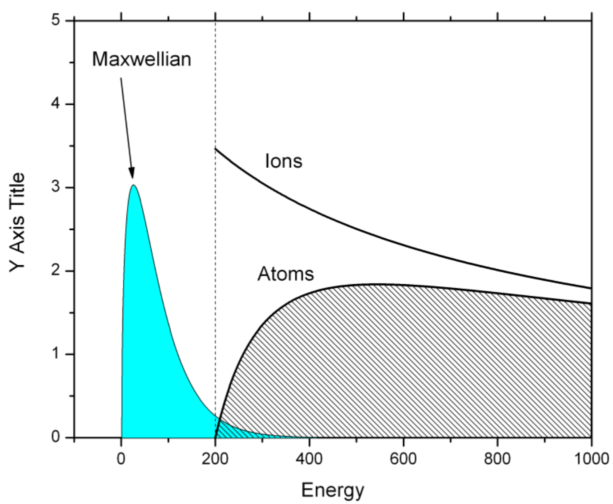
Rate coefficients for an arbitrary energy distribution function

$$\langle \sigma v \rangle = \int_{E_{min}}^{E_{max}} \sigma(E) v(E) f(E) dE \xrightarrow{Maxw} \left(\frac{8}{\pi m T^3}\right)^{1/2} \int_{\Delta E}^{\infty} E \cdot \sigma(E) \cdot e^{-E/T} dE$$

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



Often only threshold is important:



Effective collision strength:

$$\gamma(T_e) = \frac{1}{T_e} \int \Omega(E) \exp\left(-\frac{E}{T_e}\right) dE$$

$$R_{ji}(T_e) = \left(\frac{8}{\pi m T_e}\right)^{1/2} \frac{\pi a_0^2}{g_i} Ry \cdot \gamma_{ji}(T_e)$$

van Regemorter-Seaton-Bethe formula

- <u>Optically-allowed</u> excitations

Gaunt factor

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

oscillator strength

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

"*<u>Recommended</u>*" Gaunt factors:

Atoms:

$$g(\Delta n = 0, X) = \left(0.33 - \frac{0.3}{X} + \frac{0.08}{X^2}\right) \ln(X)$$

$$g(\Delta n \neq 0, X) = \left(\frac{\sqrt{3}}{2\pi} - \frac{0.18}{X}\right) \ln(X)$$

Ions:

$$g(\Delta n = 0, X) = \left(1 - \frac{1}{Z}\right)\left(0.7 + \frac{1}{n}\right)\left[0.6 + \frac{\sqrt{3}}{2\pi} \ln(X)\right]$$

$$g(\Delta n \neq 0, X) = 0.2 (X < 2), \; \frac{\sqrt{3}}{2\pi} \ln(X) \;\; for \; X \geq 2$$

Scaling of Excitations

- *n*-scaling
  - Δn=1
    - $f \sim n$, $\Delta E \sim n^{-3}$, ~~$\sigma \sim n^7$~~, $\boldsymbol{\sigma \sim n^4}$
  - Into high *n*
    - $f \sim n^{-3}$, $\Delta E \sim n^0$, $\boldsymbol{\sigma \sim \frac{1}{n^3}}$
- Z-scaling
  - Δn=0
    - $f \sim Z^{-1}$, $\Delta E \sim Z$, $\boldsymbol{\sigma \sim \frac{1}{Z^3}}$, $\boldsymbol{<\sigma v> \sim \frac{1}{Z^2}}$
  - $\Delta n \neq 0$
    - $f \sim Z^0$, $\Delta E \sim Z^2$, $\boldsymbol{\sigma \sim \frac{1}{Z^4}}$, $\boldsymbol{<\sigma v> \sim \frac{1}{Z^3}}$

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

But A ~ Z^4!!!

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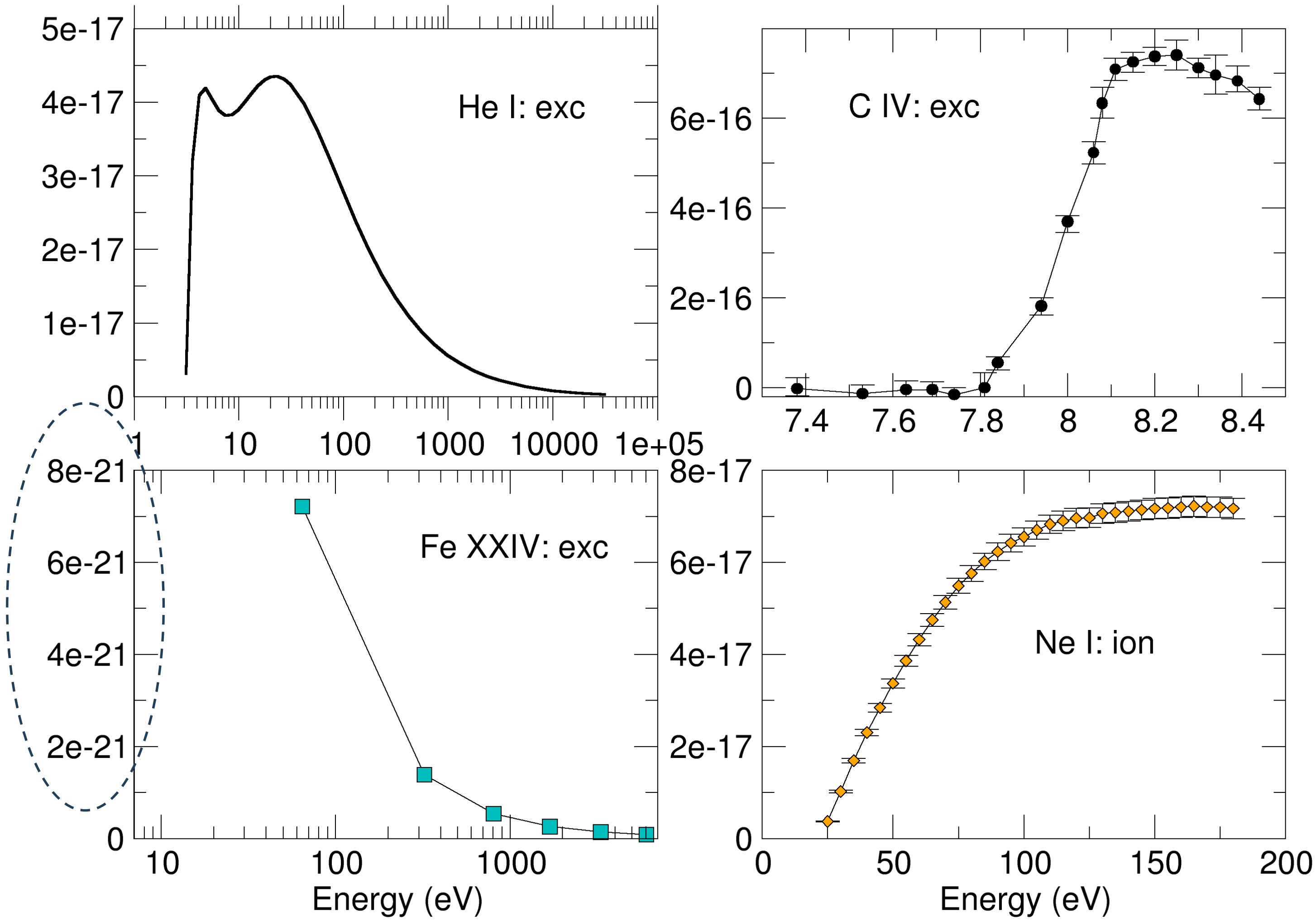
Examples: excitation and ionization (cm^2)



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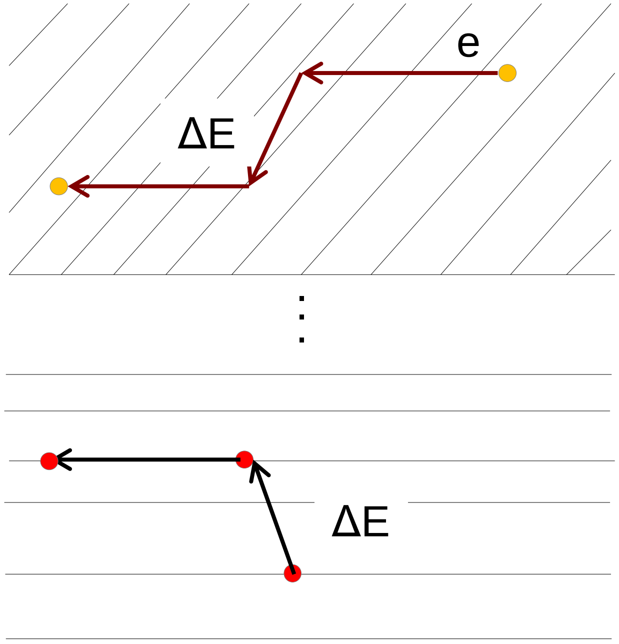
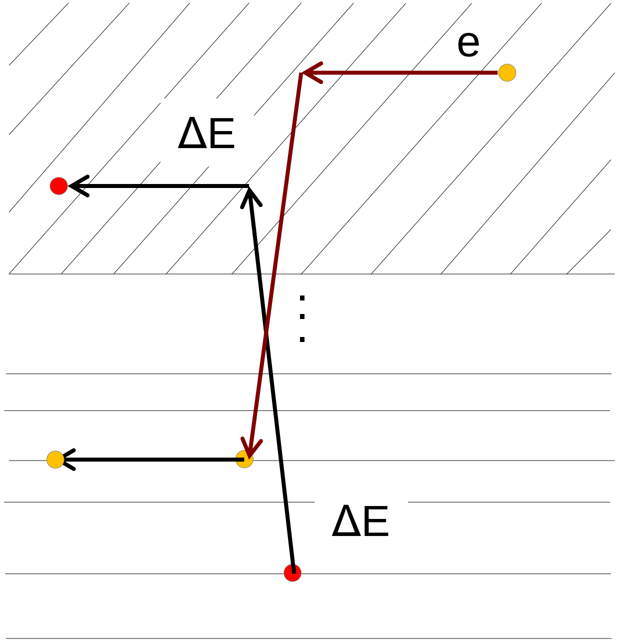
Direct and Exchange

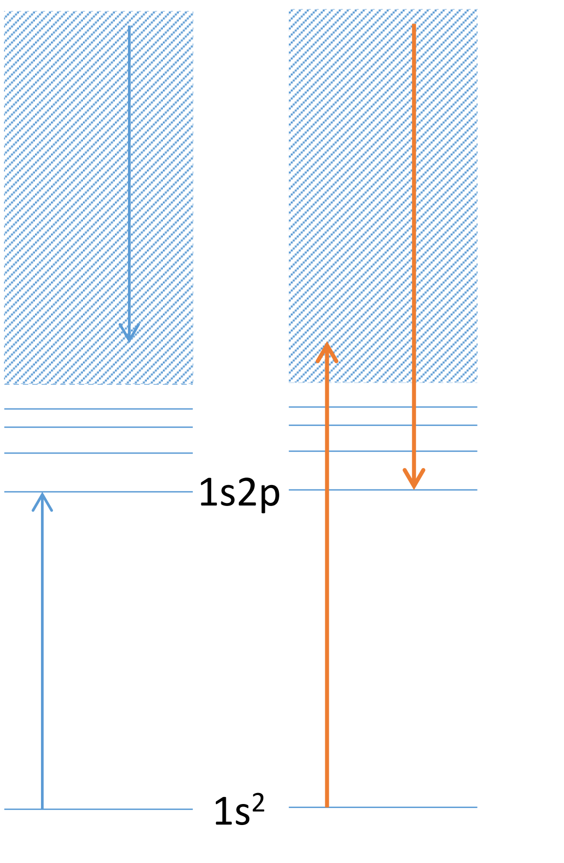
Direct channel



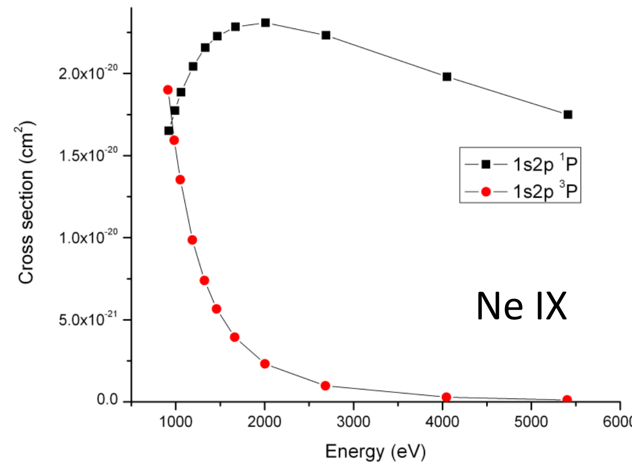
Exchange channel



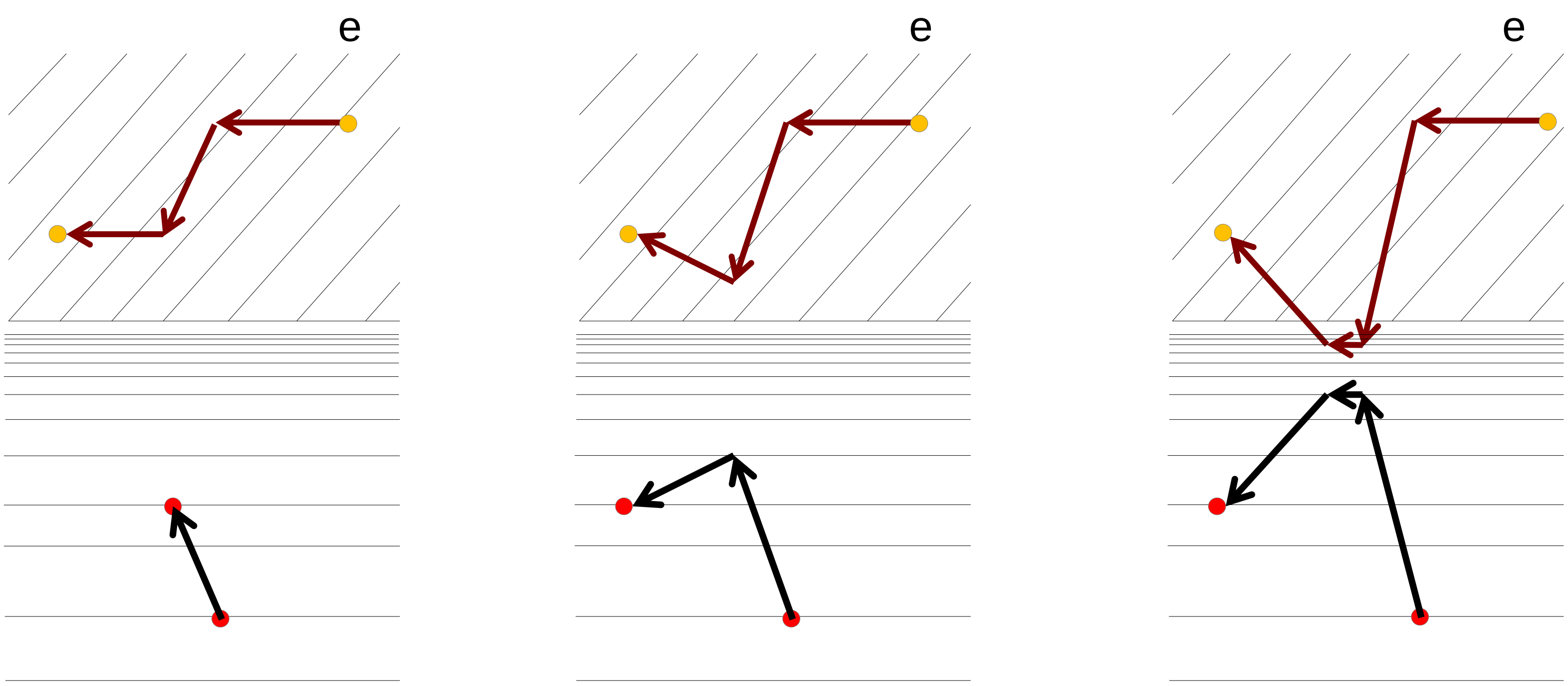
Direct and Exchange (cont'd)



He-like ion



Resonances in excitation



Direct excitation

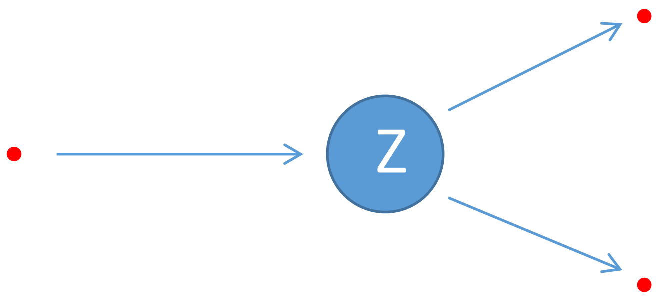
Intermediate states

Intermediate AI states

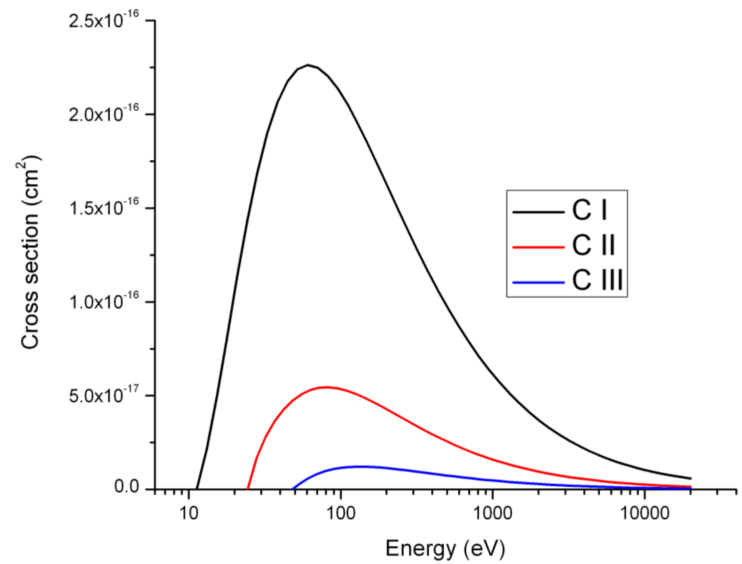
Collisional Methods and Codes

- Plane-wave Born
- Coulomb-Born (better for highly-charged ions)
- Distorted-wave method
- Close-coupling (CC) methods
  - Convergent CC (CCC)
  - R-matrix (with PS, Dirac, etc.)
  - B-splines
  - Time-Dependent CC
  - …
- Relativistic versions are available

Ionization cross sections



$$A + e \rightarrow A^{+} + e + e$$



Lotz formula:

$$\sigma_{ion}(n, E) = 2.76\pi a_0^2 \frac{Ry^2}{I_n} \frac{\ln(E/I_n)}{E} = 2.76\pi a_0^2 \frac{\boldsymbol{n^4}}{\boldsymbol{Z^4}} \frac{\ln X}{X}$$

Same theoretical methods as for excitation: Born, Coulomb-Born, DW, CC, CCC, RMPS…

3-Body Recombination

$$A + e \leftrightarrow A^{+} + e + e$$

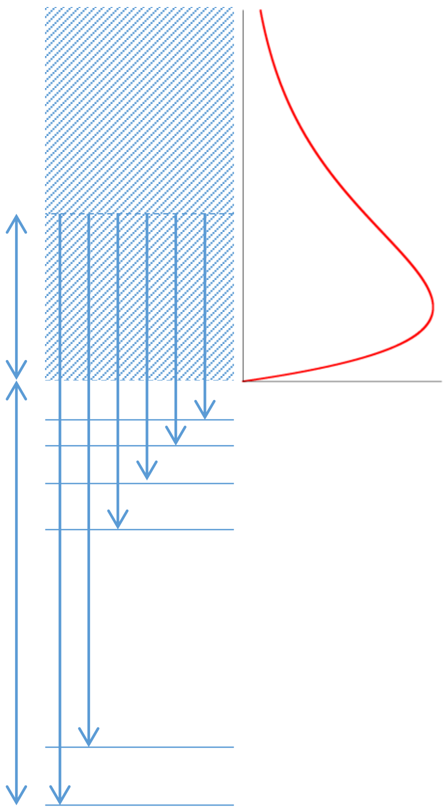
3-body rate coefficient $\alpha_{Z+1}(T_e)$ from ionization rate coefficient $S_Z(T_e)$:

$$\alpha_{Z+1}(T_e) = \frac{1}{2}\frac{g_z}{g_{z+1}}\left(\frac{2\pi\hbar^2}{m_e T_e}\right)^{3/2} exp\left[\frac{E_z}{T_e}\right] S_Z(T_e)$$

Rates from rate coefficients: $n_e S_Z(T_e)$ but $n_e^2 \alpha_{Z+1}(T_e)$

Likes high-n states; $\alpha(T_e) \sim 1/T_e^{9/2}$

Bound-free: Radiative Recombination

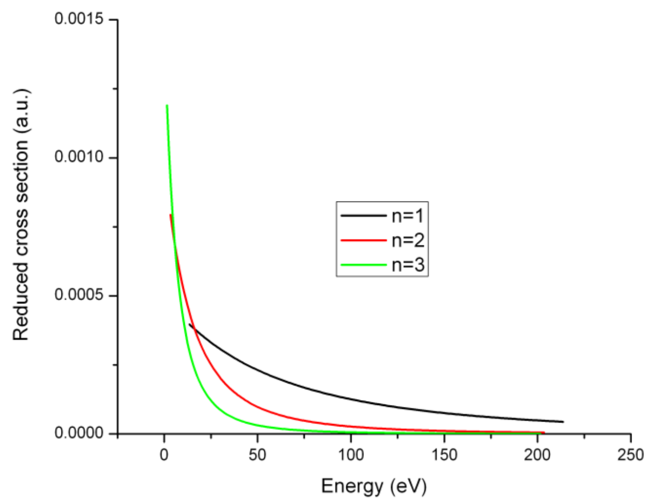


$A^{Z+} + e \rightarrow A^{(Z-1)} + h\nu$ (inverse of photoionization)

$h\nu = E + I$

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

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



Cross section Z-scaling:

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

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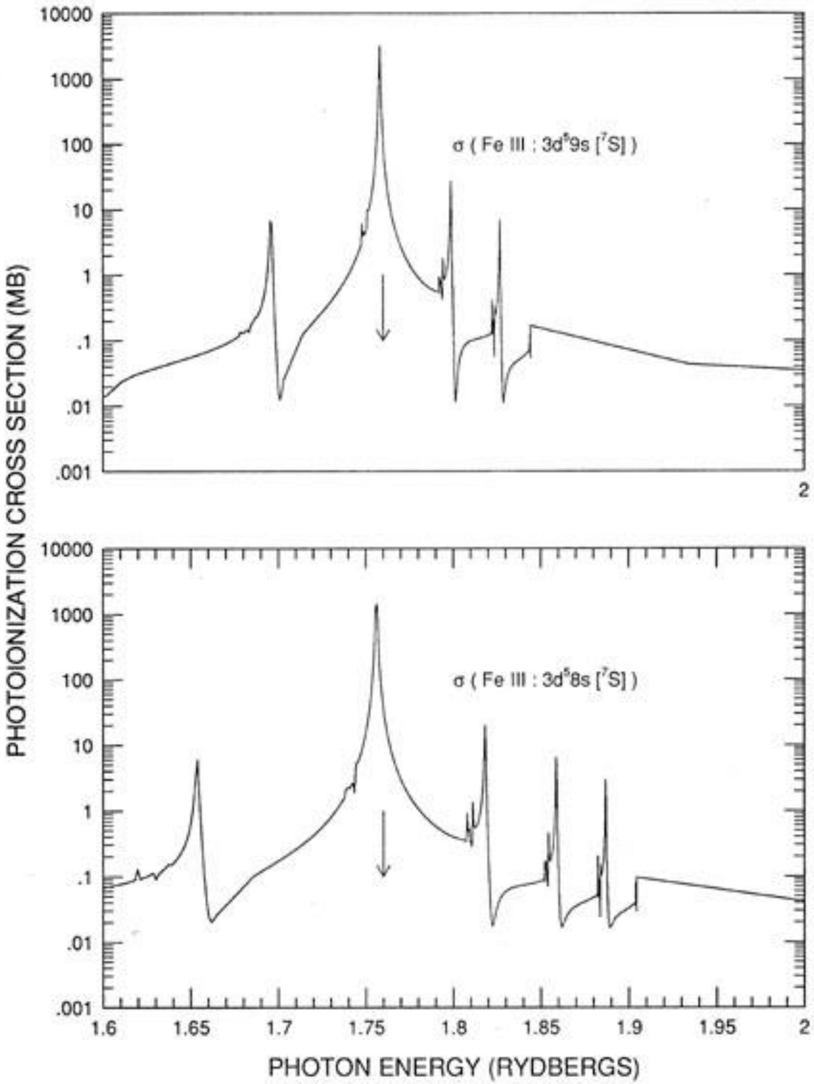
Resonances in photoionization



Fe III

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

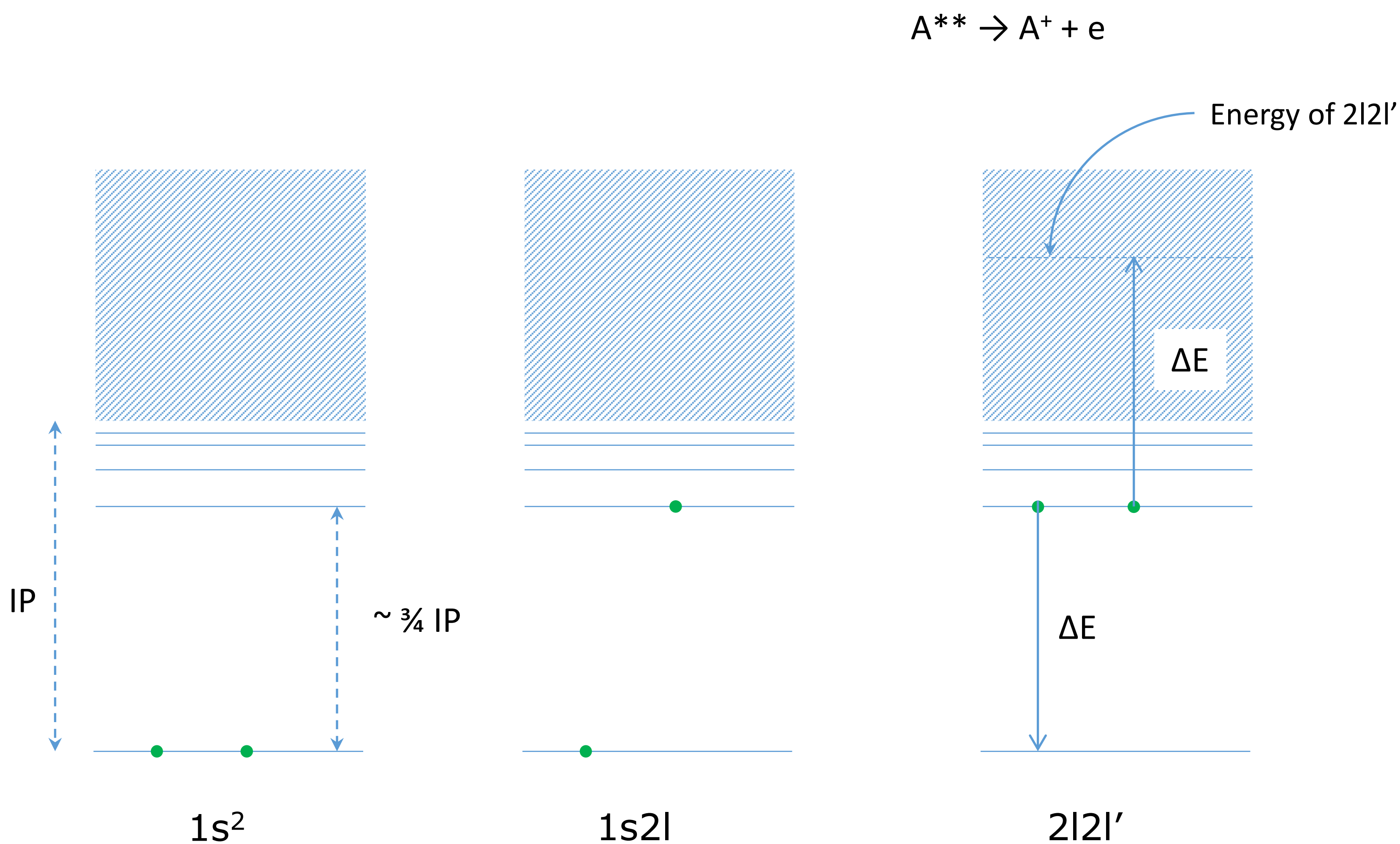
$3d^5(^6S)ns\ ^7S + h\nu$

$\rightarrow 3d^4 4p(^4P^o)ns\ ^7P^o$

$\rightarrow 3d^5\ ^6S$

A. Pradhan

Autoionization

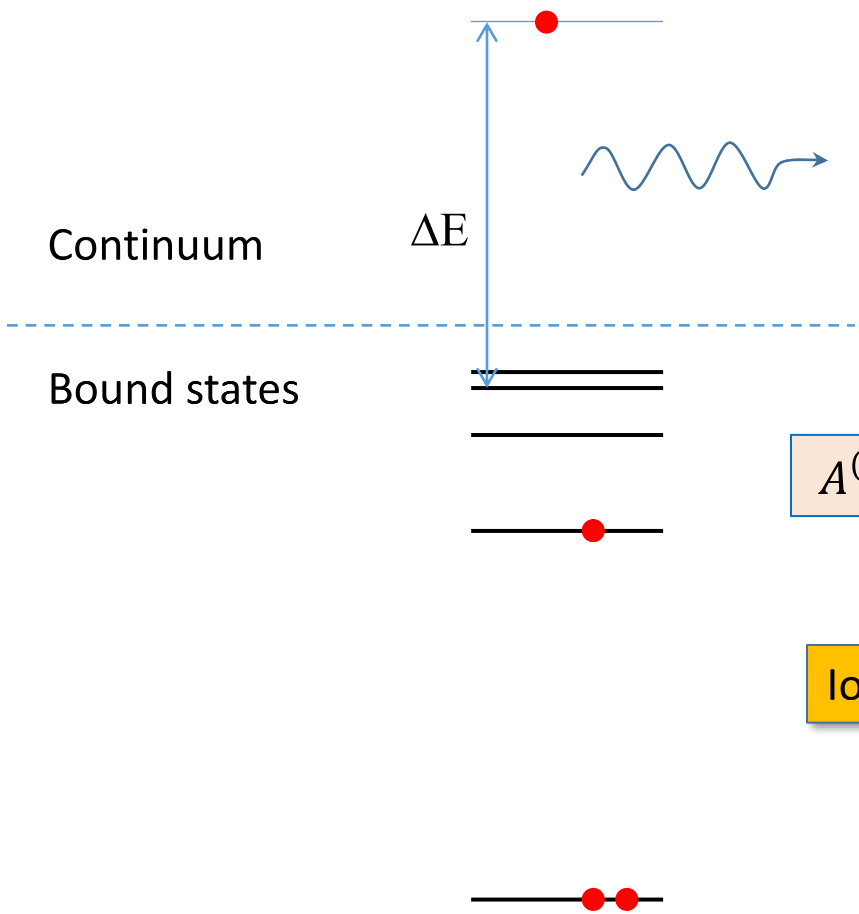


Selection rules

- Examples of AI states: $1s2s^2$, $1s^2 2pnl$ (high n)
- Typical rates: **10^{13}-10^{14} s^{-1}**
- Same old rule: before = after
- $A^{**} \rightarrow A^{*} + \varepsilon l$
  - Exact: $P_j = P_i$; $\Delta J = 0$
  - Approximate (LS coupling): $\Delta S = 0$, $\Delta L = 0$

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

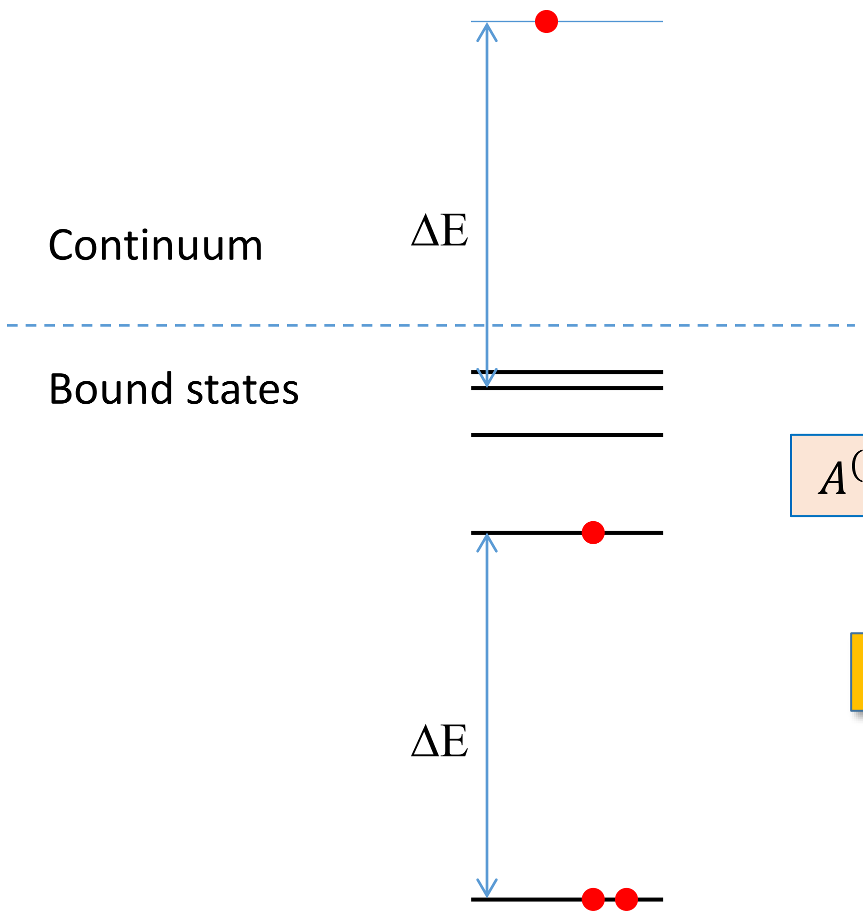
Radiative recombination



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

Ion recombined

DR step 1: dielectronic capture

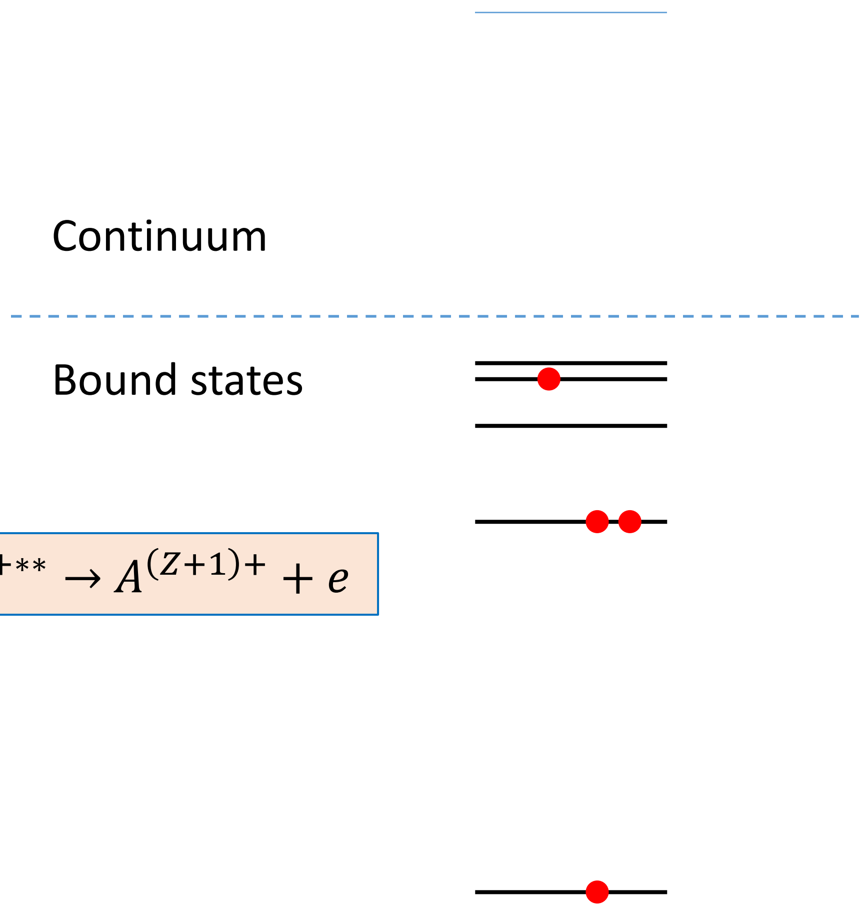


$$A^{(Z+1)+} + e \rightarrow A^{Z+**}$$

Resonant process!

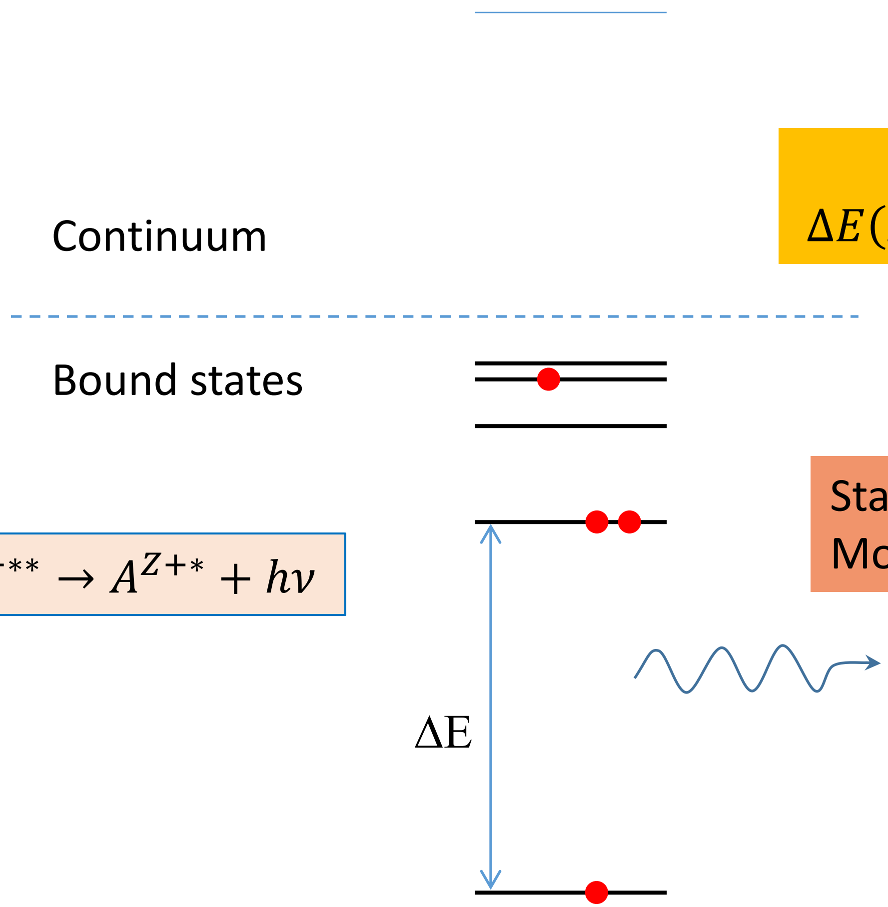
Dielectronic capture + autoionization = no recombination

DC and AI are direct and inverse



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

DR step 2: radiative stabilization



$$\Delta E(\Delta n = 0) \propto z$$
$$\Delta E(\Delta n \neq 0) \sim 13.6eV \cdot z^2$$

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

Stabilizing transition:
Mostly x-rays

Examples of dielectronic recombination & resonances

$He^+ + e$

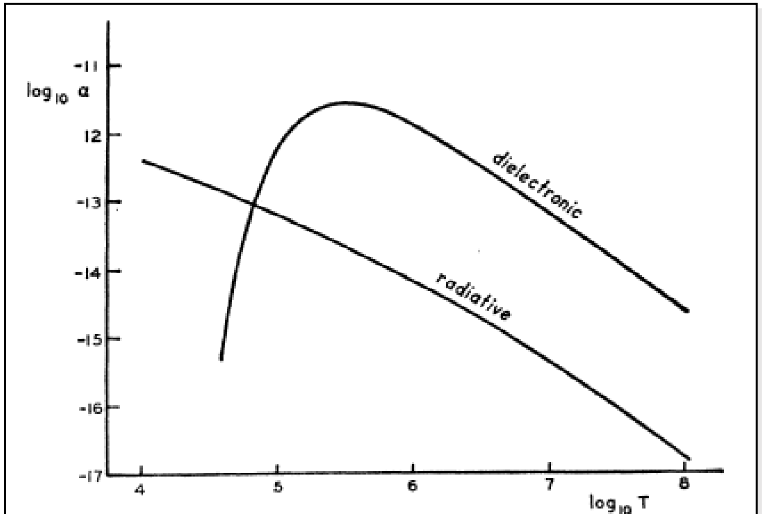
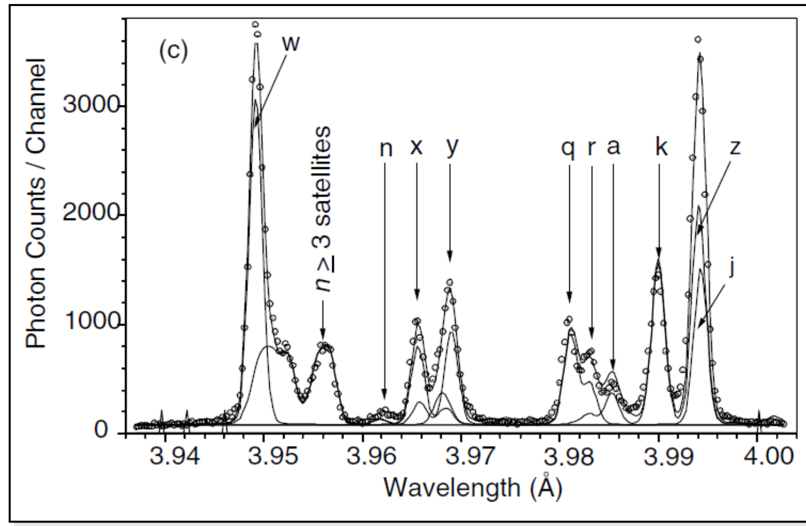


FIG 1 —$He^+ + e$ recombination coefficients α ($cm^3\ sec^{-1}$)

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)

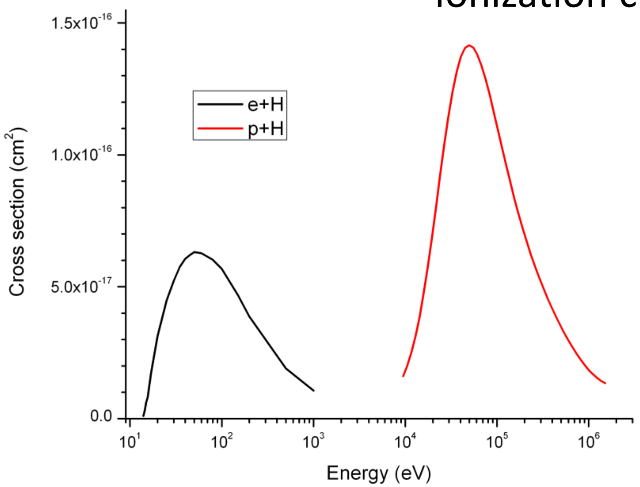


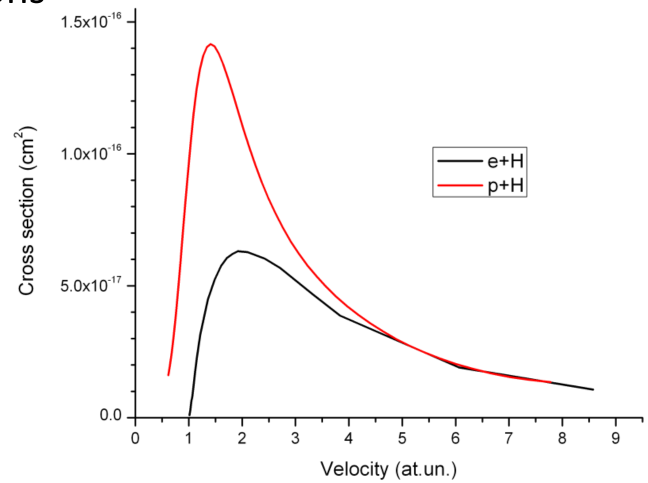
Ar at NSTX, Bitter et al (2004)

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

Heavy-particle collisions

Ionization cross sections





In ***thermal*** plasmas electrons are always more important for excitations than heavy particles
Exception: closely-spaced levels (e.g., 2s and 2p in H-like ions)

Neutral beams: **E ~ 100 keV** $\Rightarrow$ heavy particle collisions are of highest importance

Charge exchange $H + A^{z+} \Rightarrow H^{+} + A^{(z-1)+}(n)$

- Very large cross sections **> 10^{-15} cm^2**; $\sigma(Z) \sim Z \cdot 10^{-15}\ cm^2$
- High excited states populated: **$n \sim Z^{0.77}$**
- Higher l values are preferentially populated but it depends on collision energy

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