Mechanisms of departures from LTE

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‘Mechanisms of departures from LTE’

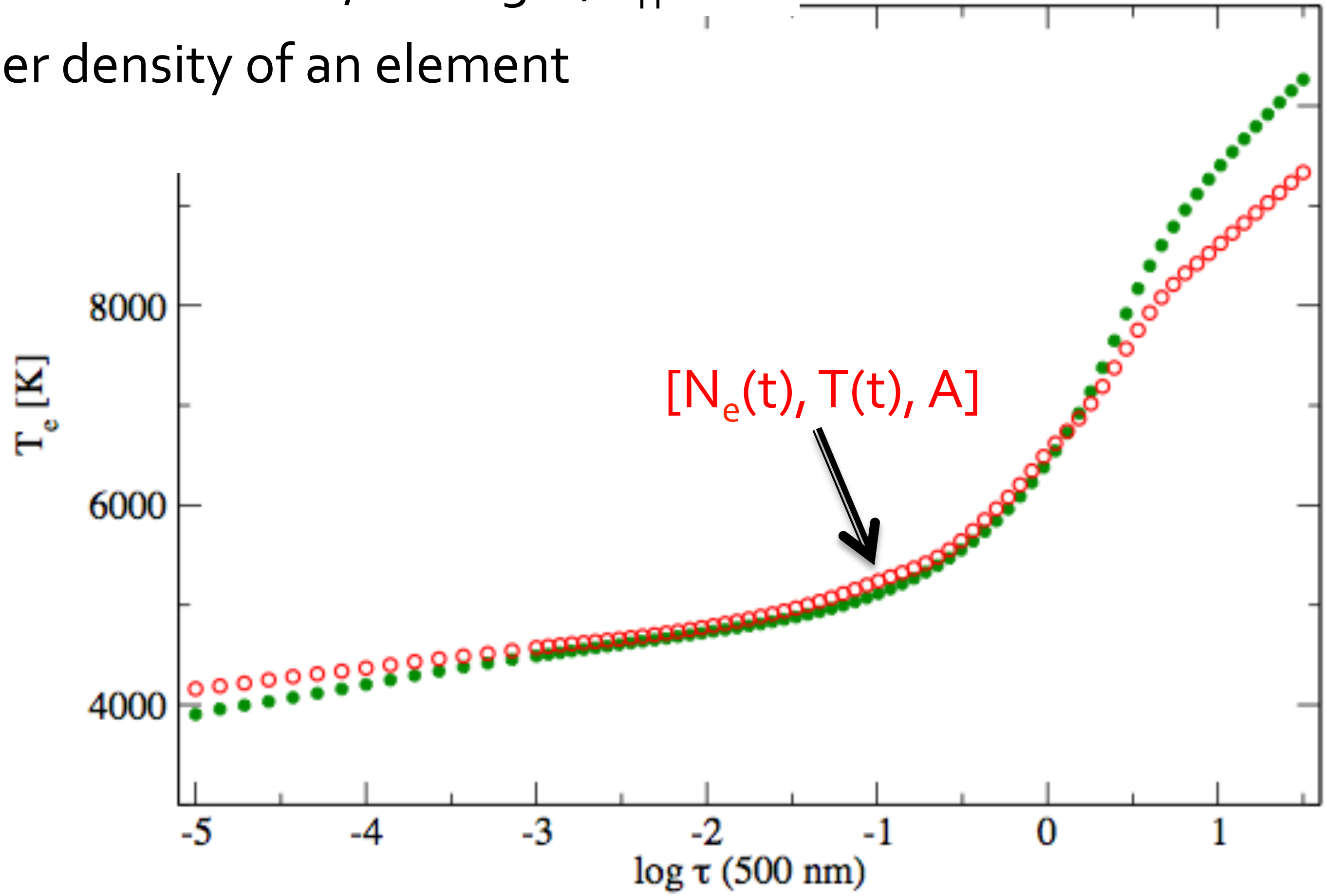
processes which trigger deviations of atomic level populations from the LTE values

What is NLTE? → what is LTE

Assumption: level populations are what they will be given the local values T, N_e, A

A – abundance of an element, $A = \log N/N_H + 12$

N - total number density of an element [atoms /cm^3]

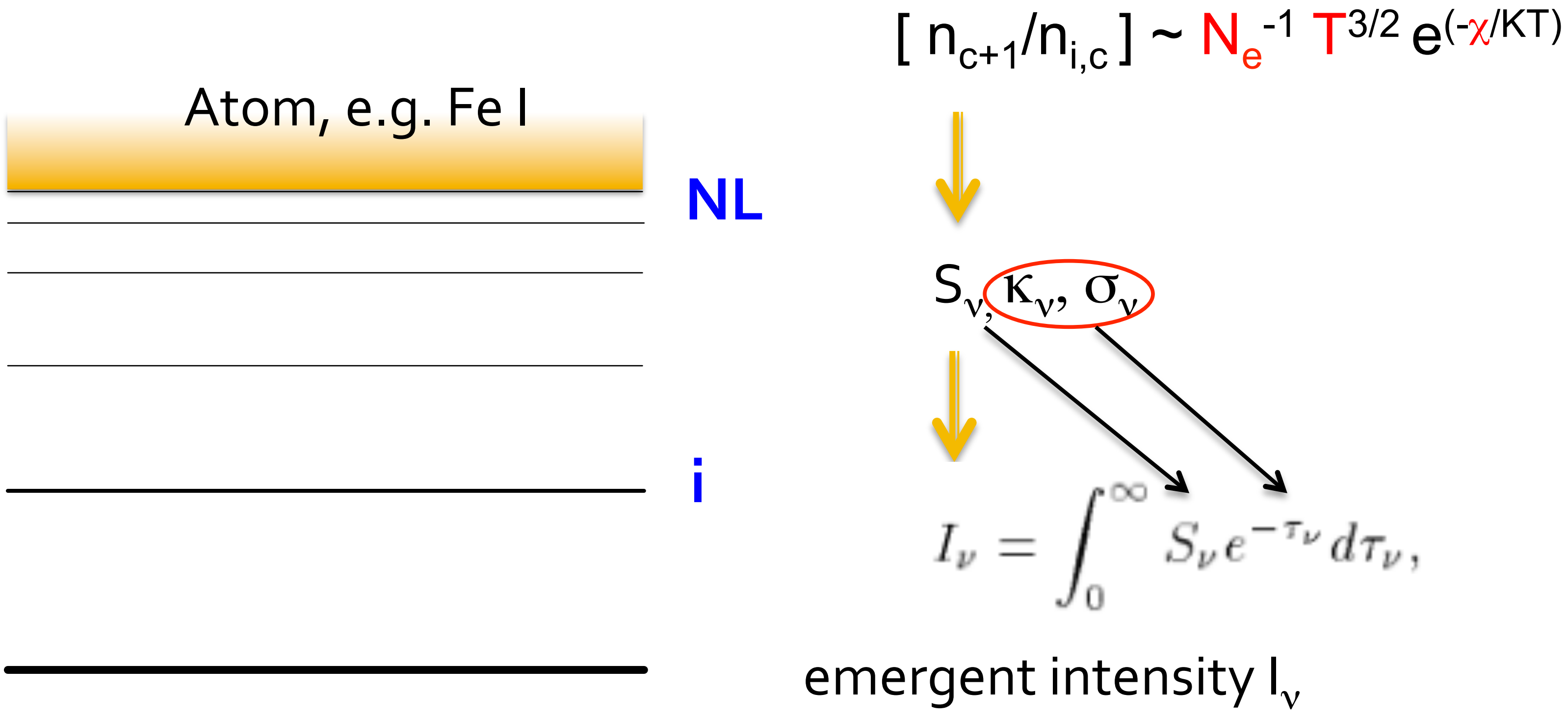


$[N_e(t), T(t), A]$

LTE

We neglect transitions in the atom caused by radiation

$n_{i,c}$ – level population, [atoms /cm^3]
χ – ionization energy of an ion



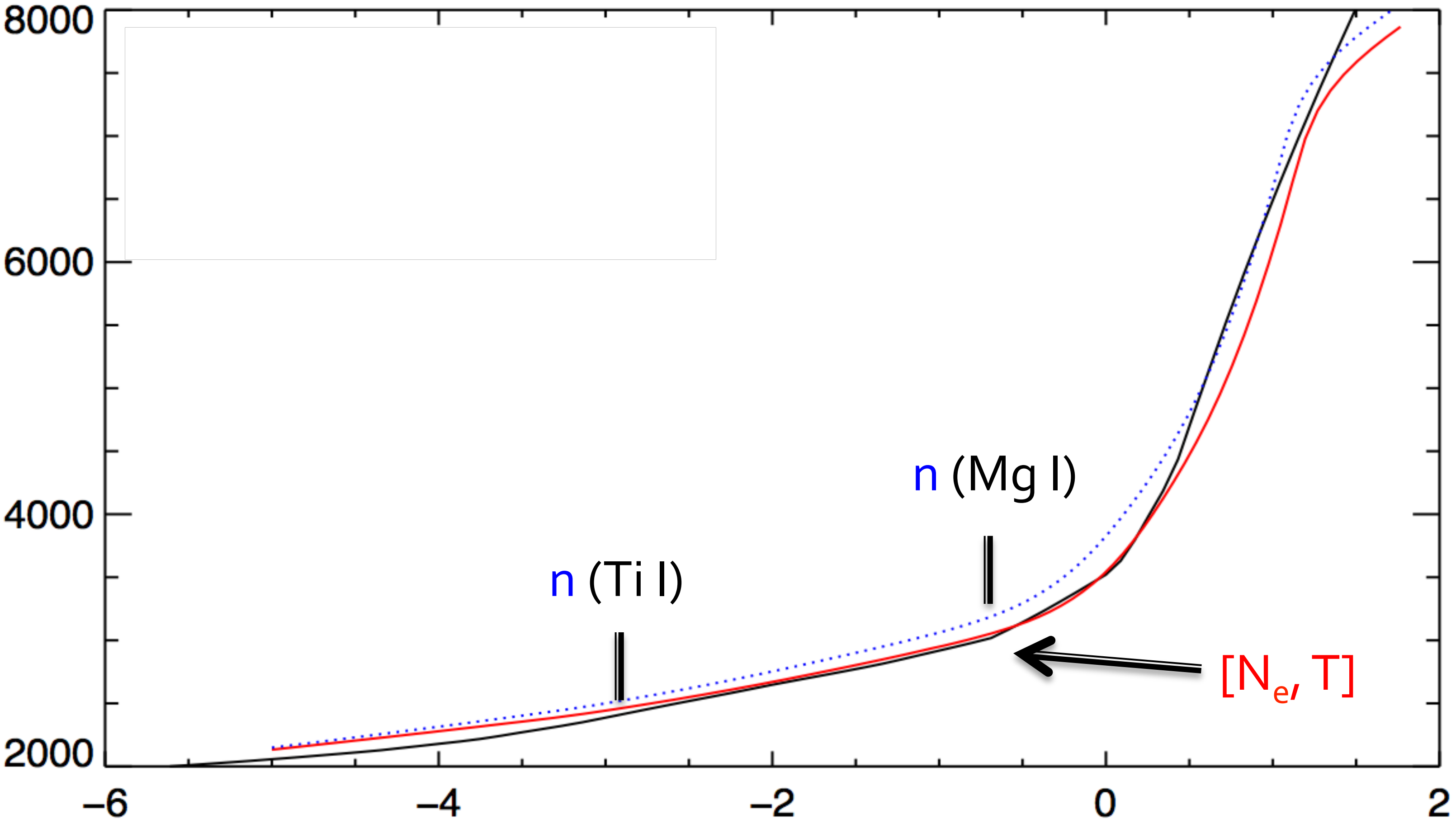
$$[\, n_{c+1}/n_{i,c} \,] \sim N_e^{-1}\, T^{3/2}\, e^{(-\chi/KT)}$$

$$S_\nu, \kappa_\nu, \sigma_\nu$$

$$I_\nu = \int_0^\infty S_\nu e^{-\tau_\nu} d\tau_\nu,$$

emergent intensity I_ν

LTE: line formation is coupled to the local temperature and density

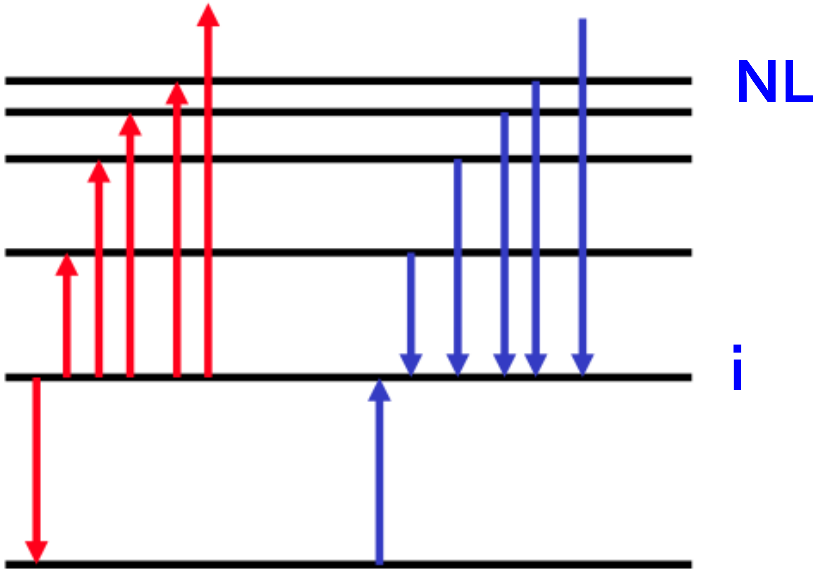


NLTE: statistical equilibrium

$$n_i \sum (C_{ij} + R_{ij}) = \sum n_j (C_{ji} + R_{ji}), \quad i = 1, \ldots, NL$$

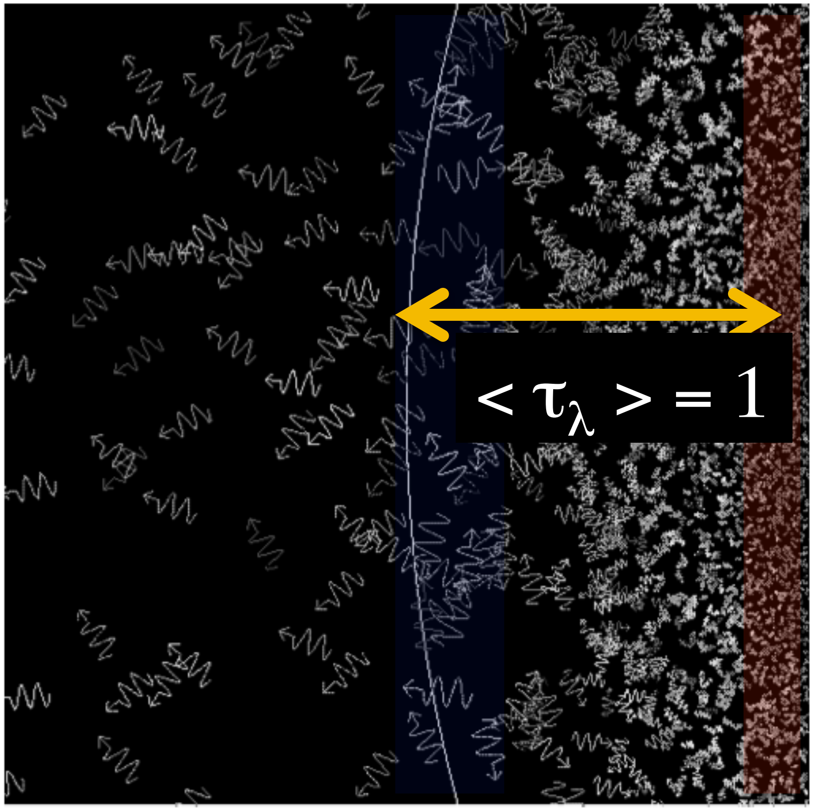
Rates out = Rates in

C_{ij}, R_{ij} – transition rates [1/second/particle]



Statistical equilibrium
the number of atoms in each excitation level i and each ionization stage j

Photosphere: a transition from LTE to extreme NLTE



Extreme NLTE

LTE:
Saha-Boltzmann equations for calculation of atomic number densities

Departures from LTE = NLTE

caused by the radiation field that departs from the isotropic blackbody radiation field (J_ν /= B_ν) characteristic of the local T_e

Strong interdependence between the properties of material (κ_ν, σ_ν) and the radiation field (I_ν) !

$$N_i \sum (C_{ij} + R_{ij}) = \sum N_j (C_{ji} + R_{ji}) \quad i = 1, \ldots, NL \qquad \textbf{(1)}$$

«Rates» of transitions [1/sec/particle]:

$R_{ij} = B_{ij} J_\nu$ (b-b)

$R_{ic} = 4\pi \int k_\nu J_\nu \, d\nu / h\nu$ (b-f)

↓

LTE if $J_\nu = B_\nu(T)$

or $C_{ij} \gg R_{ij}$

$$\mu \, dI_\nu/dz = -\alpha_\nu I_\nu + \varepsilon_\nu \qquad \textbf{(2)}$$

$\alpha_\nu, \varepsilon_\nu = F(N_i)$

Equations (1) and (2) must be solved simultaneously!

↓

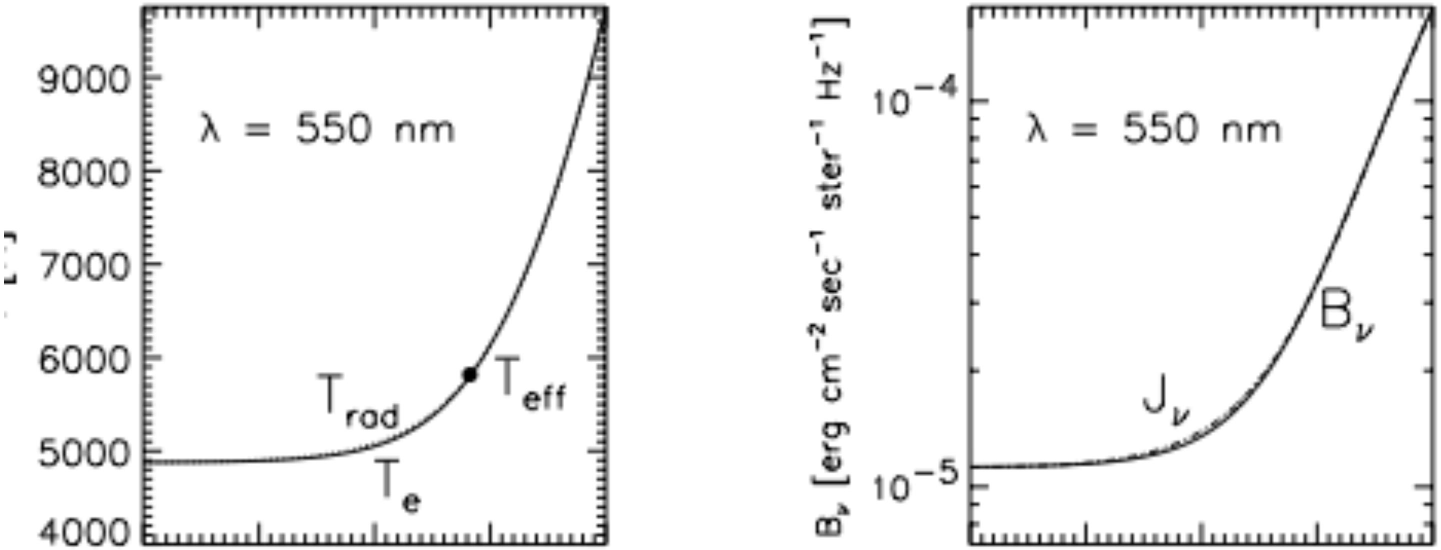
N_i

LTE if $J_\nu = B_\nu(T)$

or $C_{ij} \gg R_{ij}$

Are these conditions satisfied in FG stars?

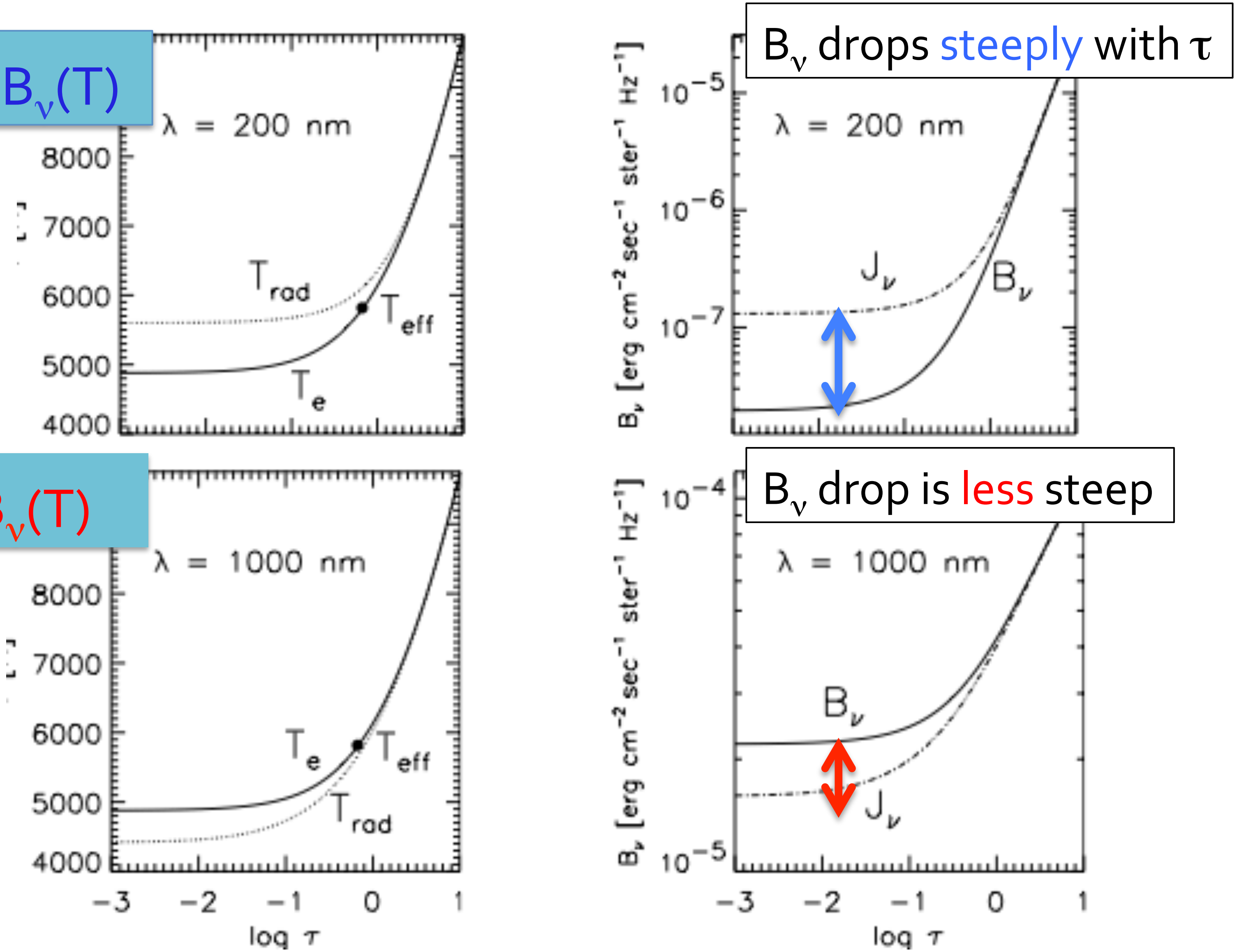
$J_\nu = B_\nu(T)$ at 500 nm



T_{rad} = Te

R. Rutten (lecture notes)

But, $J_\nu \neq B_\nu(T)$ at other frequencies even **in LTE**

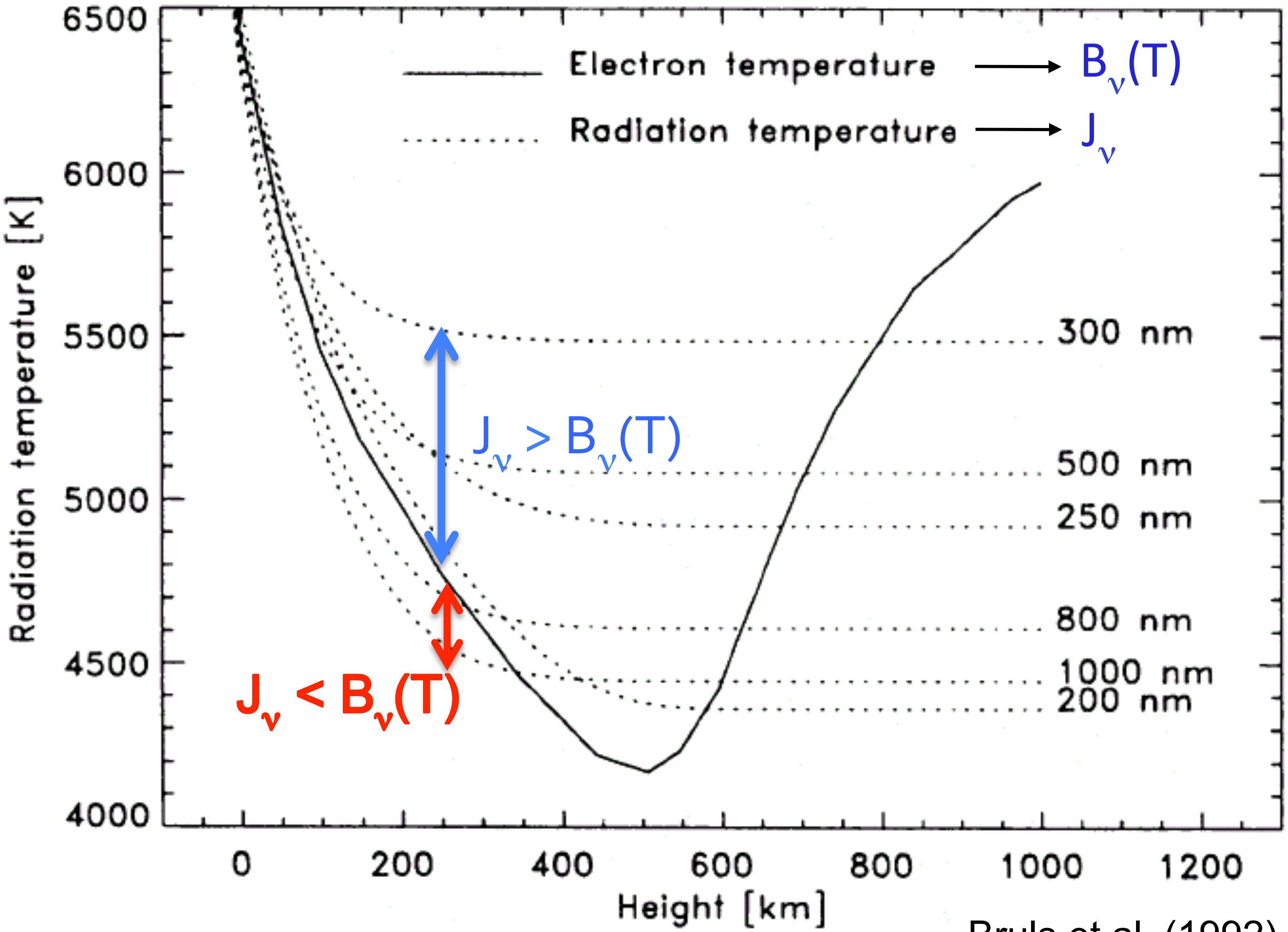


UV: $J_\nu > B_\nu(T)$

B_ν drops steeply with τ

IR: $J_\nu < B_\nu(T)$

B_ν drop is less steep



$B_\nu(T)$

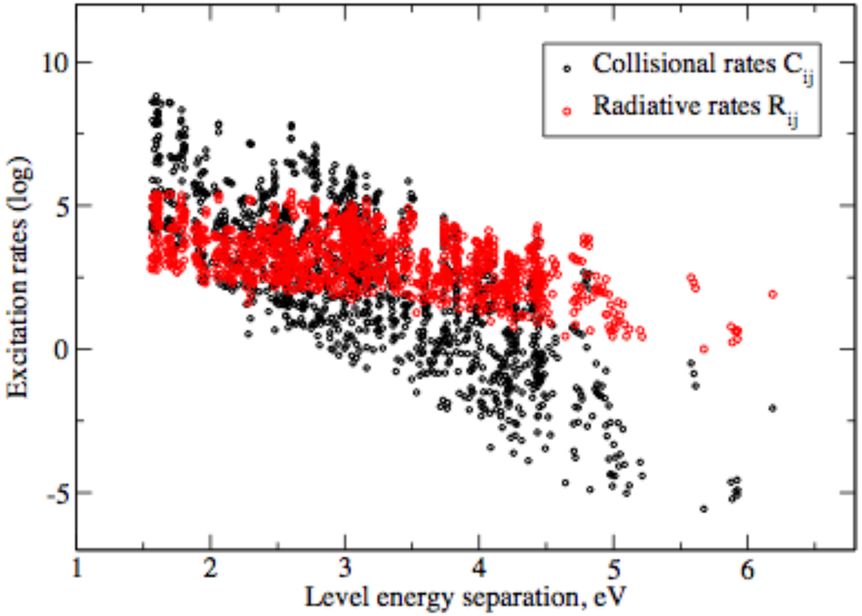
J_ν

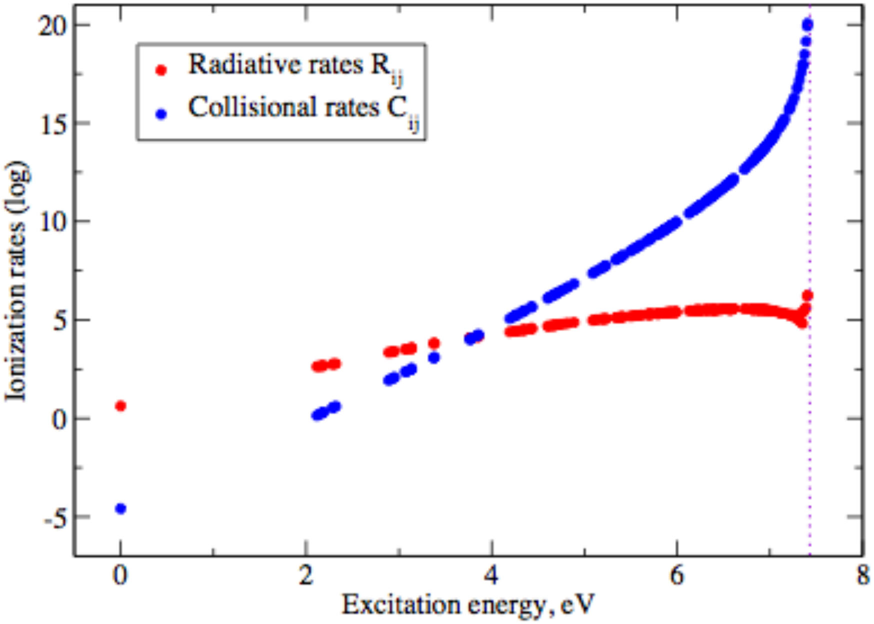
$J_\nu > B_\nu(T)$

$J_\nu < B_\nu(T)$

Bruls et al. (1992)

The rates for the Fe I atom in a model of a solar atmosphere

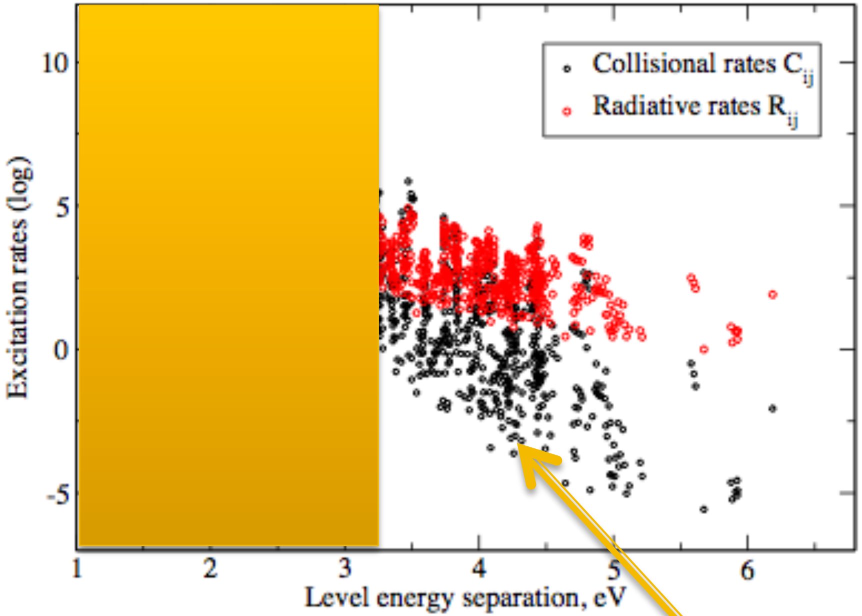


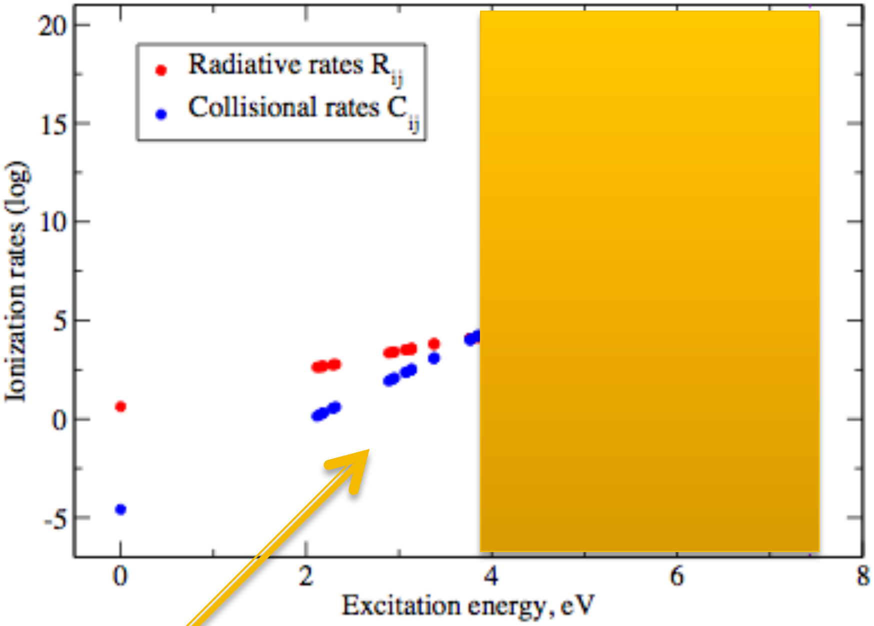


C_{ij} (coll rates) /= R_{ij} (radiative rates)

Bergemann (2008)

The rates for the Fe I atom in a model of a solar atmosphere





The levels and transitions important for the exc-ion. balance of Fe I

R_{ij} (radiative rates) are LARGER than C_{ij} (coll rates)

LTE if $J_\nu = B_\nu(T)$

or C_{ij} » R_{ij}

The conditions are not satisfied in FG stars

$$\sum_{n>m} N_n\left(A_{nm}+B_{nm}J_\nu+C_{nm}\right)+\sum_{k<m} N_k\left(B_{km}J_\nu+C_{km}\right)+N_\mathrm{e}\left(R_m+Q_m\right)$$
$$-N_m\left\{\sum_{k<m}\left(A_{mk}+B_{mk}J_\nu+C_{mk}\right)+\sum_{n>m}\left(B_{mn}J_\nu+C_{mn}\right)+\left(P_m+S_m\right)\right\}=0$$

Radiative (photo-) ionization *P*
Radiative recombination *R*

$$P_m = 4\pi\int\frac{a_\nu J_\nu}{h\nu}d\nu$$

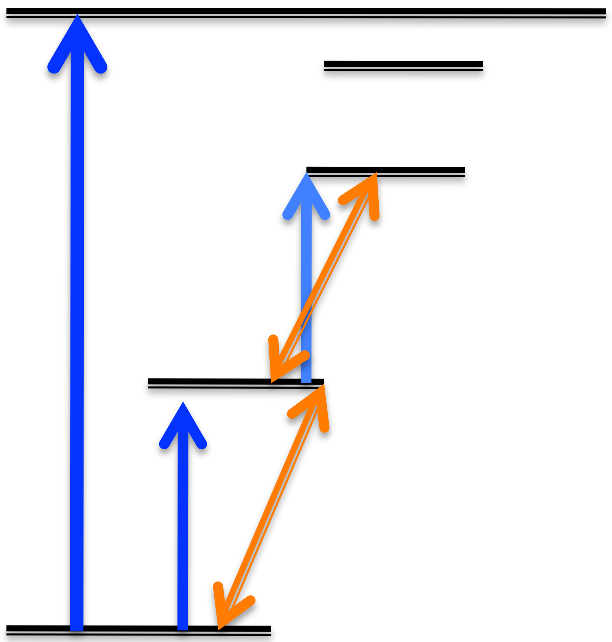
Collisional ionization *S*
Collisional recombination *Q*

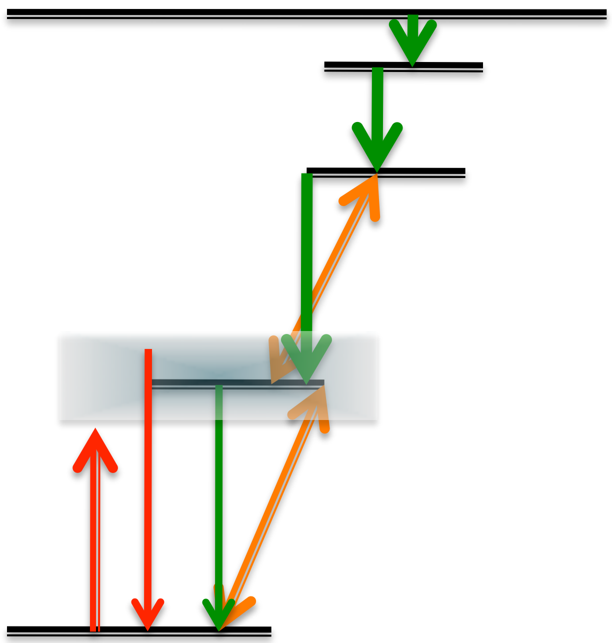
Radiative emission A_{nm}
Stimulated emission B_{nm}

NLTE mechanisms

1. over-ionization
2. photon pumping
3. IR over-recombination
4. photon suction
5. photon loss in resonance lines

not unique physical processes, but **mechanisms that describe** how **statistical equilibrium is achieved**





Overionization

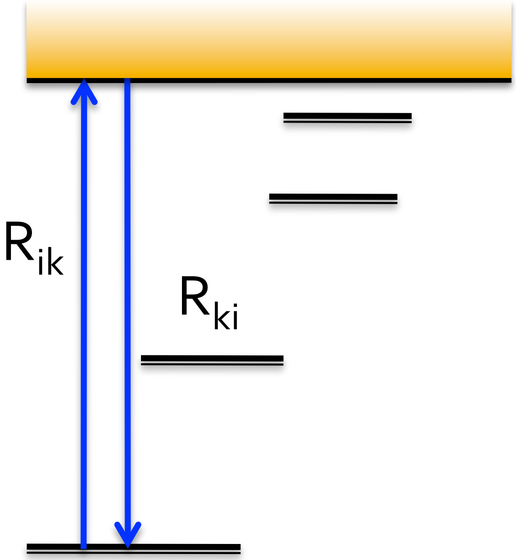
R: [transitions/sec/particle]

$$R_{ik} \sim \int \frac{\sigma_\nu J_\nu}{h\nu} d\nu$$

radiative ionization

$$R_{ki} \sim B_\lambda(T_e)$$

radiative recombination



ν_{ik} – frequency of a level ionization edge

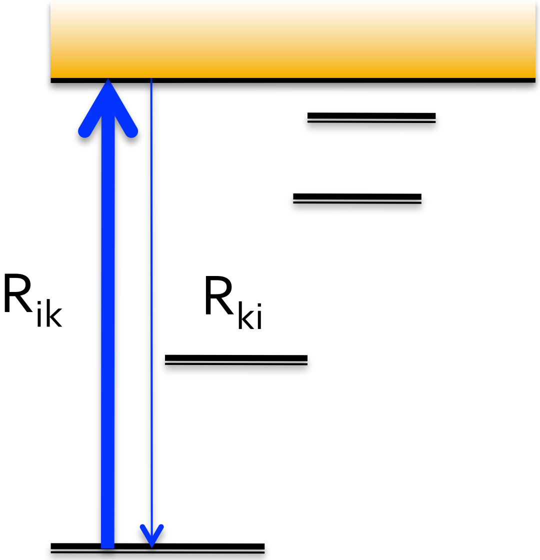
σ_{ik} – ionization cross-section
(from lab. experiments and/or
theoretical quantum-mechanical
calculations)

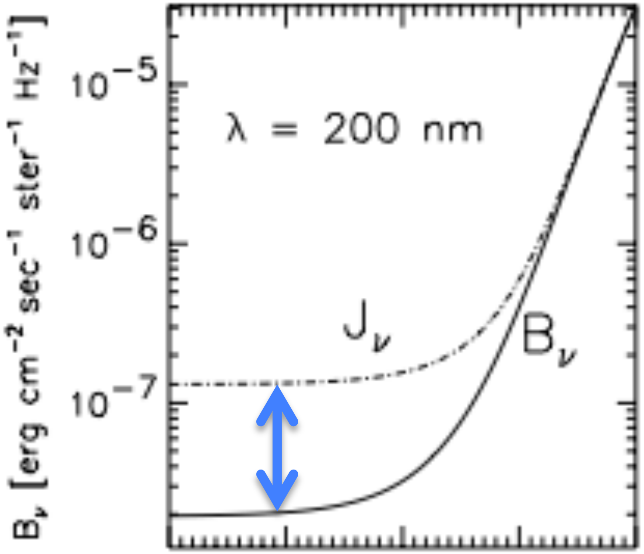
Overionization

R: [transitions/sec/particle]

$$R_{ik} \sim \int \frac{\sigma_\nu J_\nu}{h\nu} d\nu$$ radiative ionization

$$R_{ki} \sim B_\lambda(T_e)$$ radiative recombination





J_ν drops less steeply than $B_\nu(T)$ in the UV

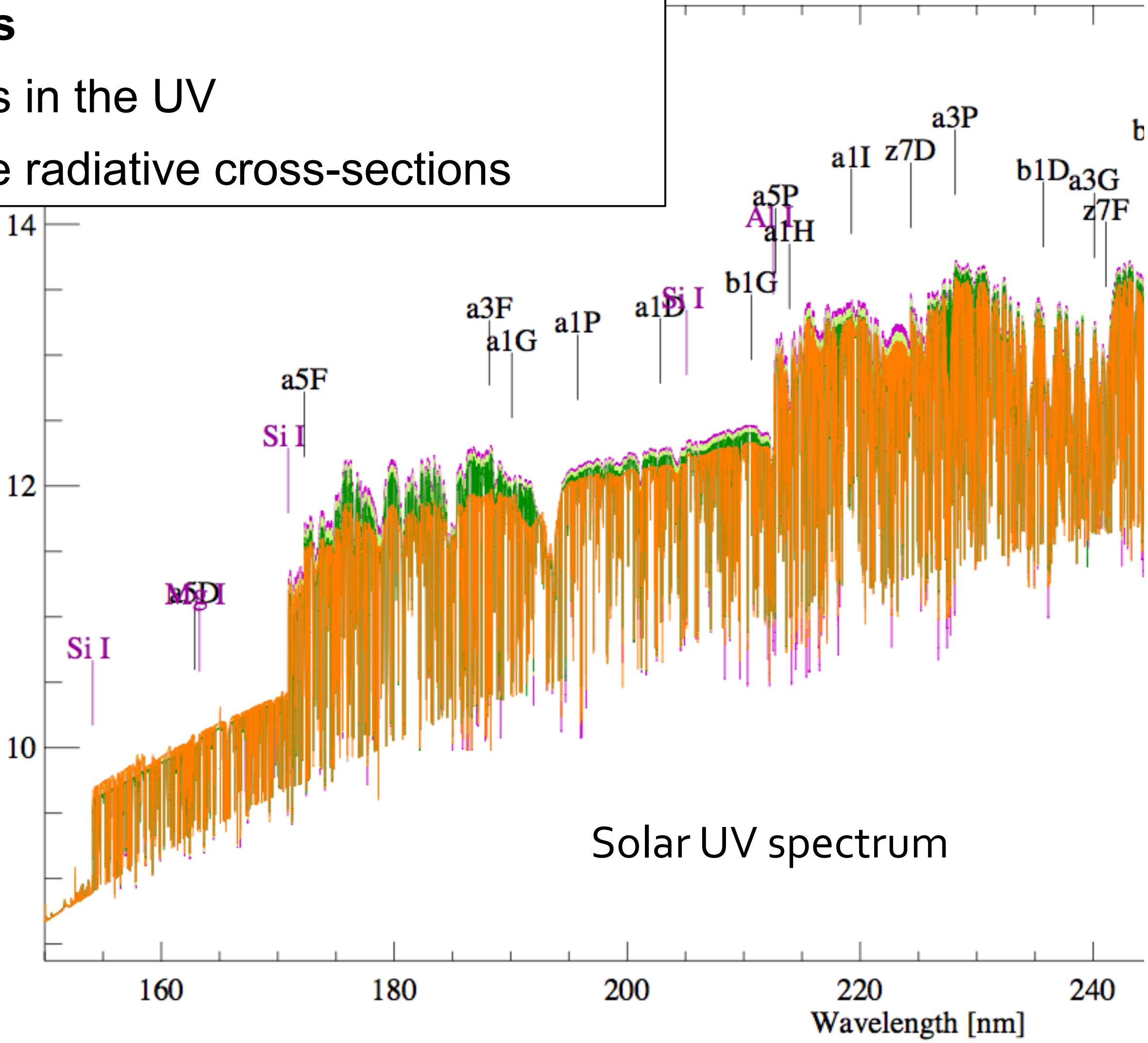
$J_\nu >> B_\nu(T)$ ➡ $R_{ik} >> R_{ki}$

Rate out > Rate in

Overionization

Neutral minority atoms

- with ionization edges in the UV
- and large bound-free radiative cross-sections

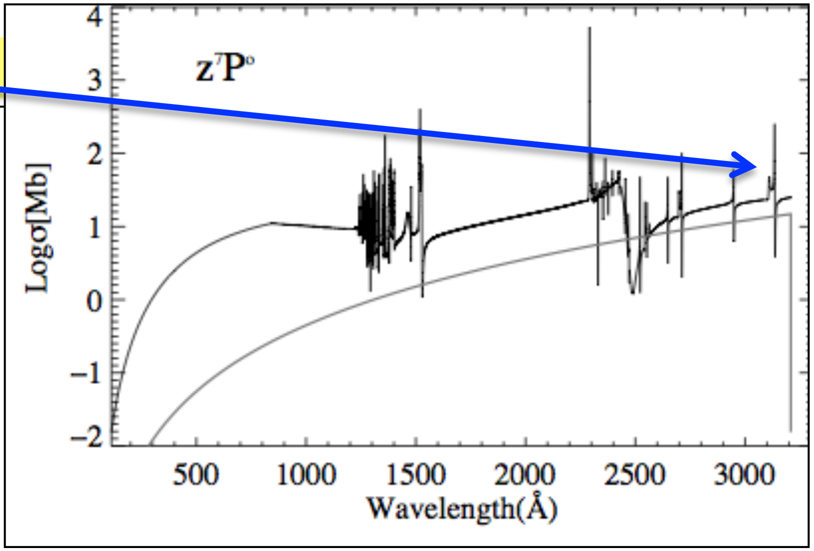


Solar UV spectrum

Atoms with large *bound-free* absorption edges (an atomic property)

Ion	Level	l_0 [nm]	a_0 [MBarn]
H I	$n = 2$	364.7	15.84
Mg I	3s ^{1}S	162.1	1.18
	3p ^{3}P^o	251.4	20.00
	3p ^{1}P^o	375.7	11.95
Al I	3p ^{2}P^o	207.1	65.00
Si I	3p ^{3}P	152.1	39.16
	3d ^{1}D^o	168.2	34.49
	4s ^{1}S^o	198.6	33.56
Fe I	a^{5}D	156.9	4.06
Cr I	z^{7}P	320.1	13.3

Mg I, Al I, Si I,
Fe I, Cr I, Ti I
Mn I, Co I, Ni I
…

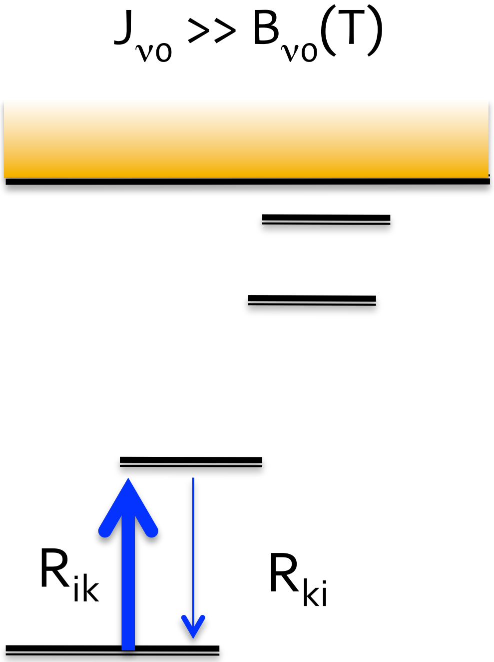


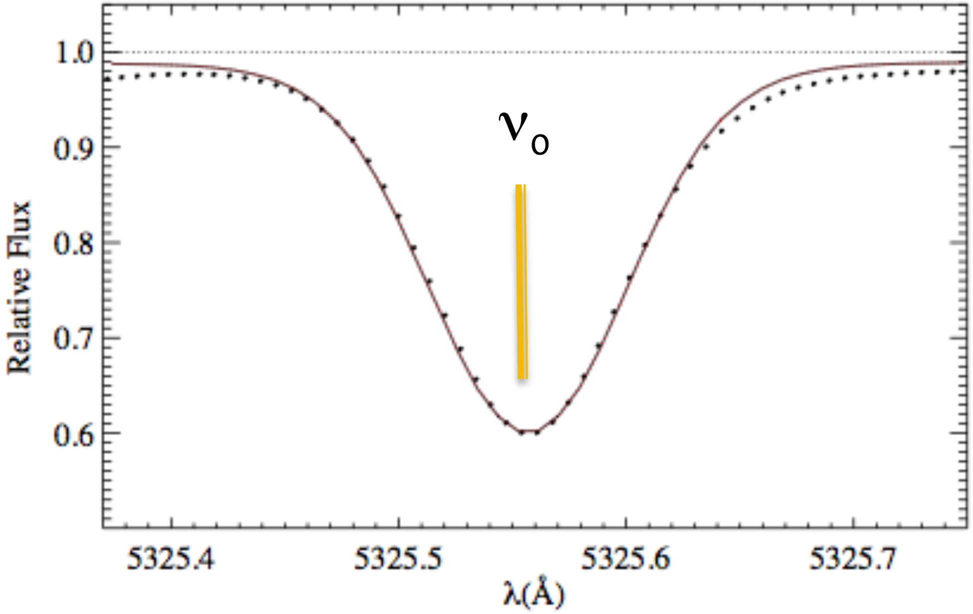
Fe I has a large number of *bf* absorption edges between 200 and 300 nm

Photon pumping

A transition is ‘pumped’ if:

- opacity is large in the line core ($\tau_{\nu o} > 1$)
- line wings are transparent ($\tau_{\nu} < 1$)





The same as radiative ionization but at the frequencies of line transitions

Photon suction

$$R_{ik} \sim \int \frac{\sigma_\nu J_\nu}{h\nu} d\nu$$

radiative ionization

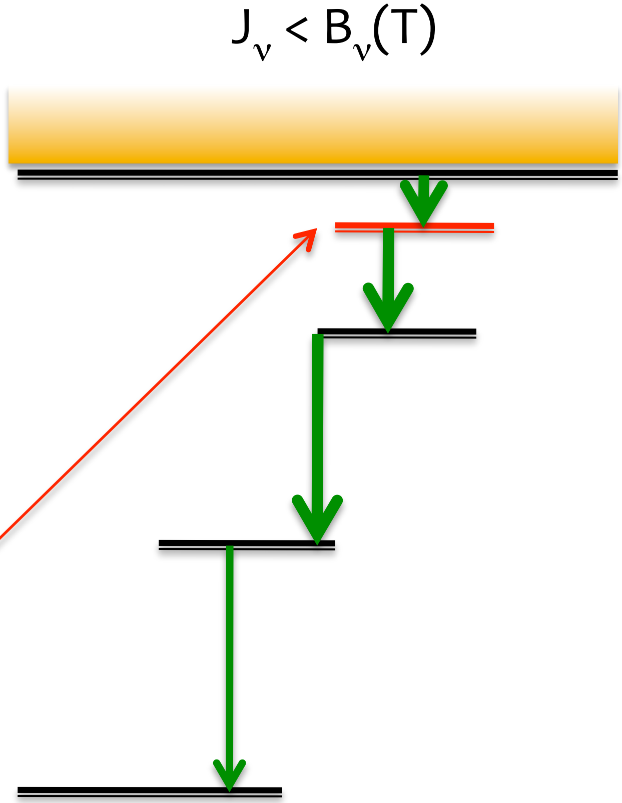
radiative recombination

$$R_{ki} \sim B_\lambda(T_e)$$

J_ν drops below $B_\nu(T)$ in the (Infra)-red when radiative equilibrium holds

↓

Recombination in the bound-free edges of high-excitation levels (inverse of over-ionization)

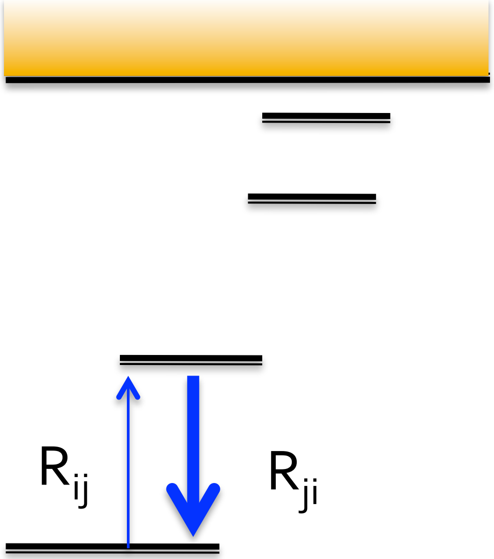


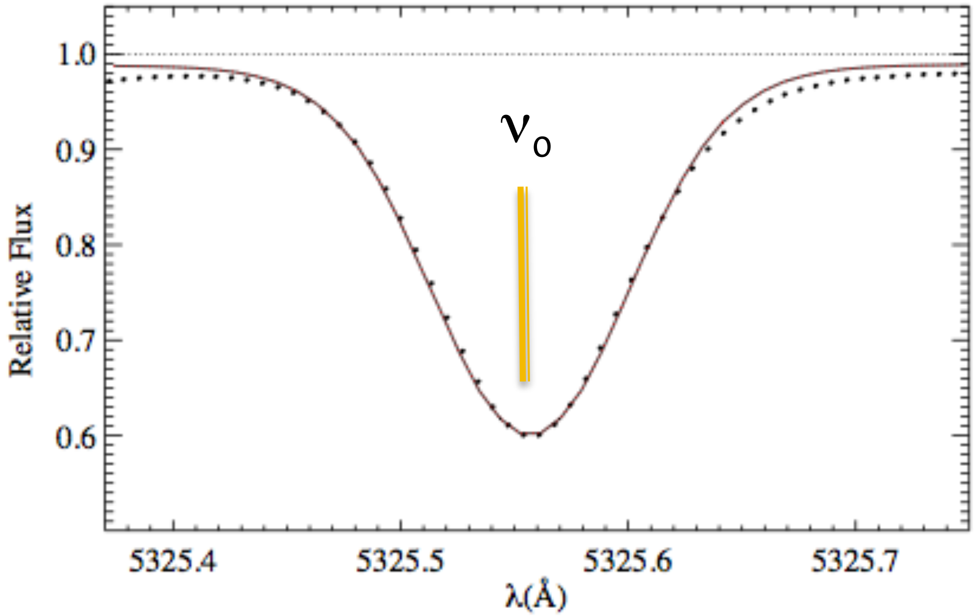
Photon loss

opacity is small in the line core ($\tau_{\nu o} < 1$), too less photo-excitations

→ photons ‘escape’

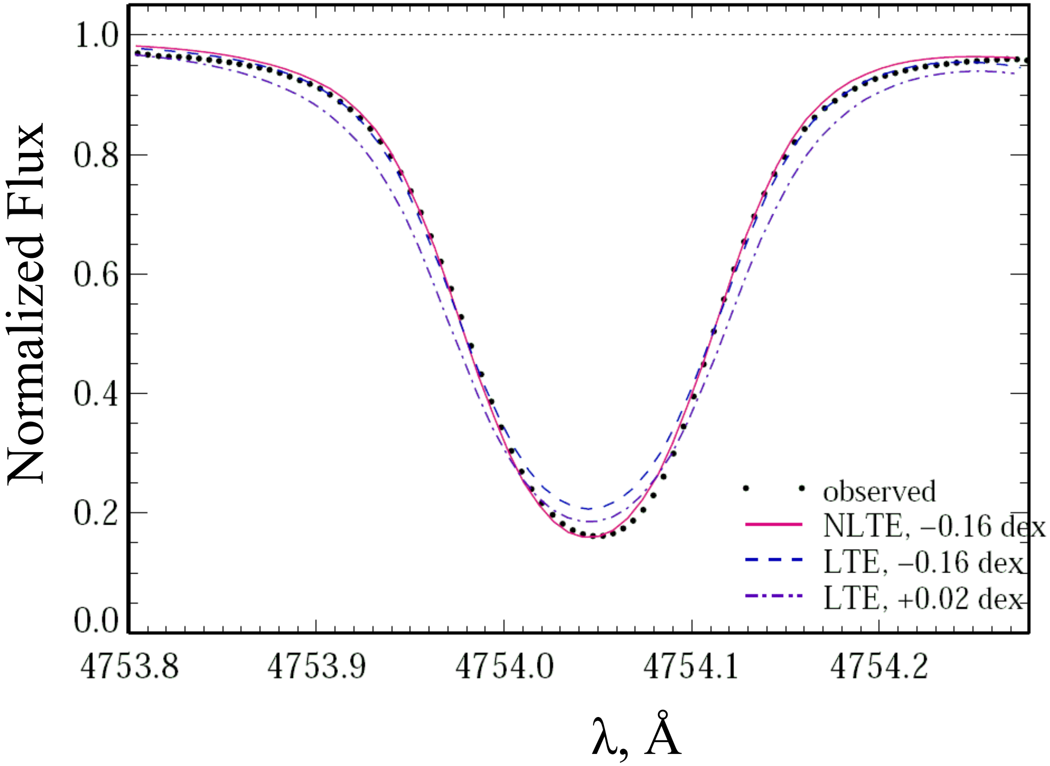
$J_{\nu o} < B_{\nu o}(T)$

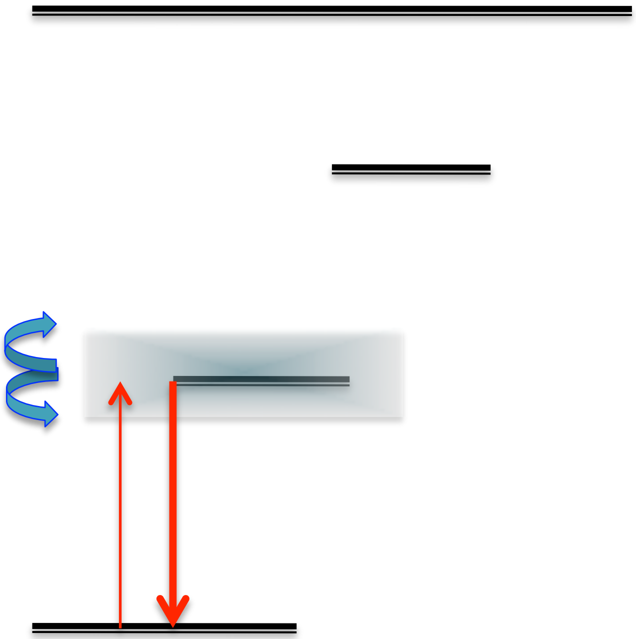




Resonance line scattering and photon loss

Due to frequency redistribution in the line profile, a photon can escape in the wings from far below the location, where $\tau_{\nu o} <= 1$.





Deviations from LTE

in most cases, all these NLTE effects are present

The type and magnitude of a **dominant** NLTE effect depend on:

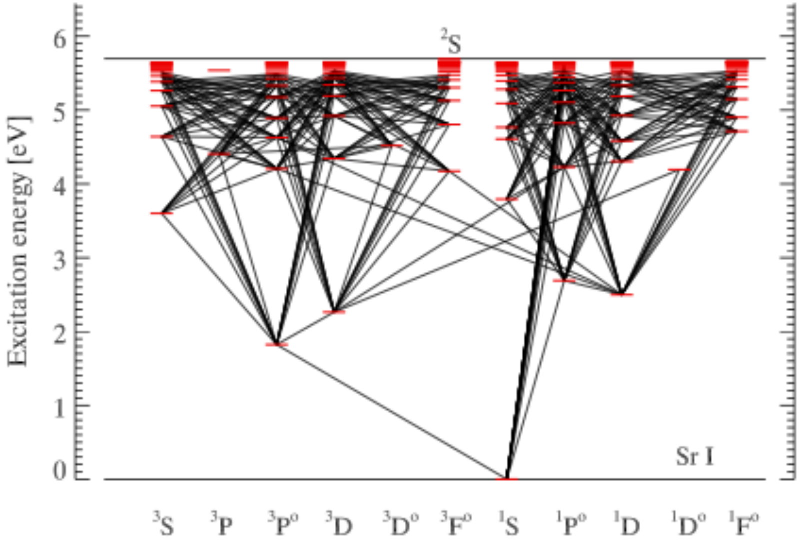
- *physical conditions* (T, log g, [Fe/H]) in the atmosphere
- *atomic structure*

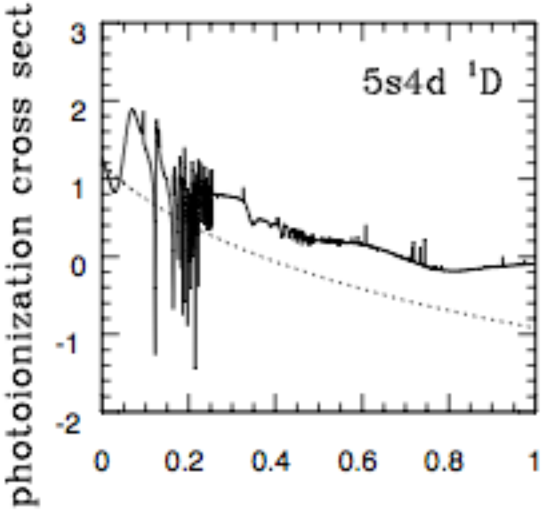
Deviations from LTE

Atomic structure

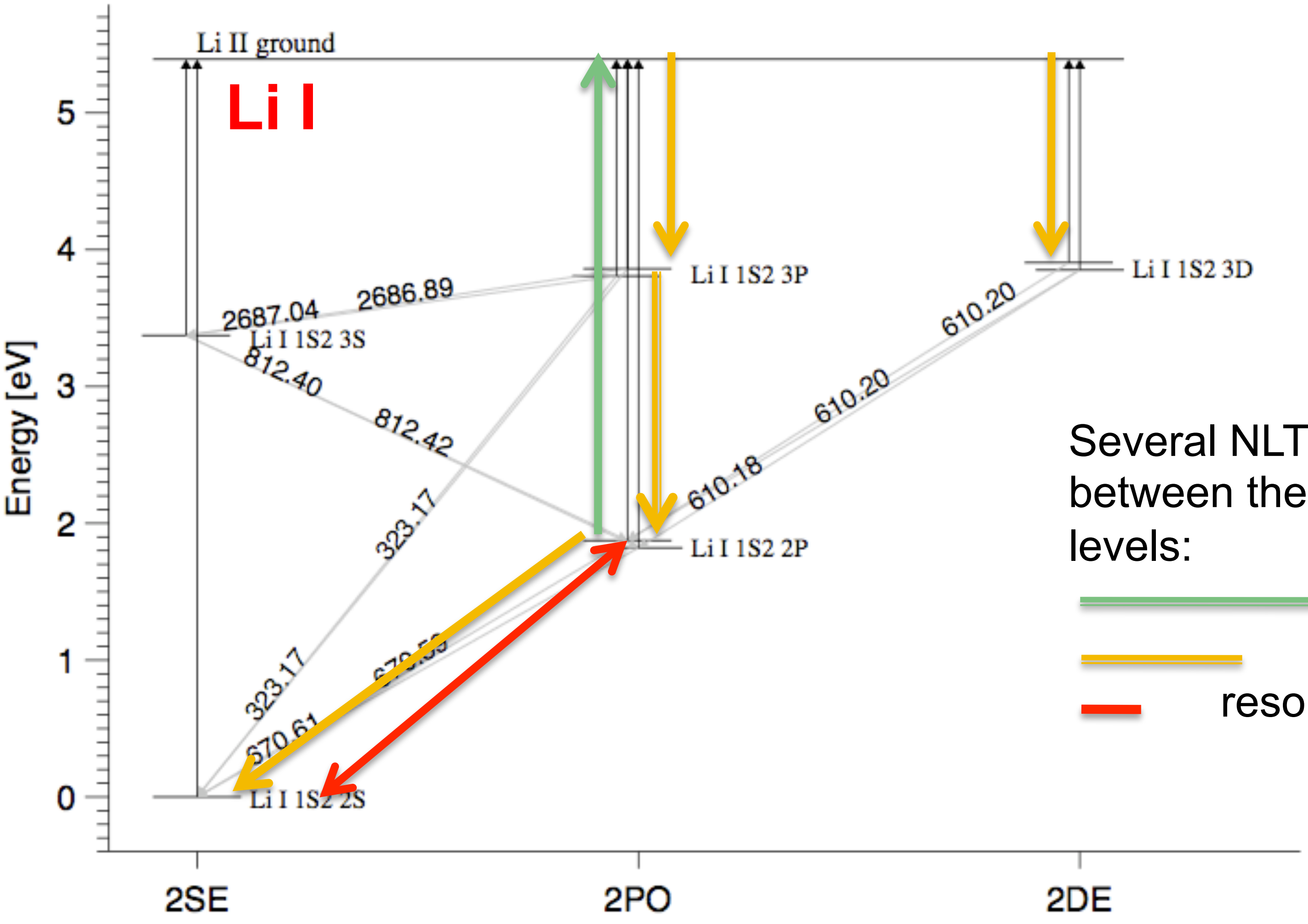
- ionization energy, which gives relative abundances [Fe I/ Fe II] depending on the T/log g
- characteristics of energy levels in the atom
- number of transitions (allowed, forbidden)
- magnitude of cross-sections for particle interactions

(f-values, photoionization, H I and e impact excitation and ionization, di-electronic recombination, charge transfer)





Light elements



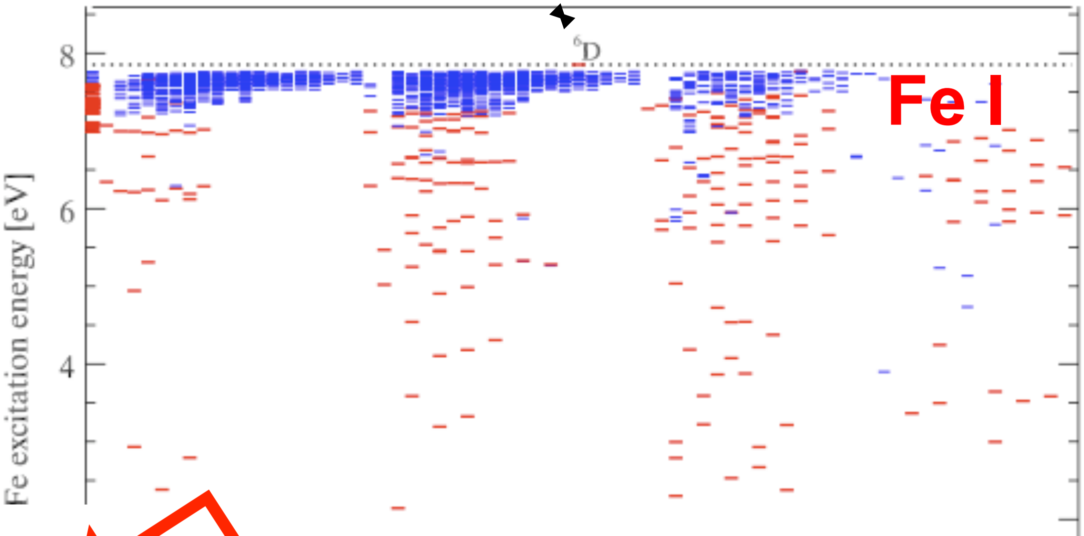
Several NLTE processes act between these **9 Li I** energy levels:

🟩 overionization

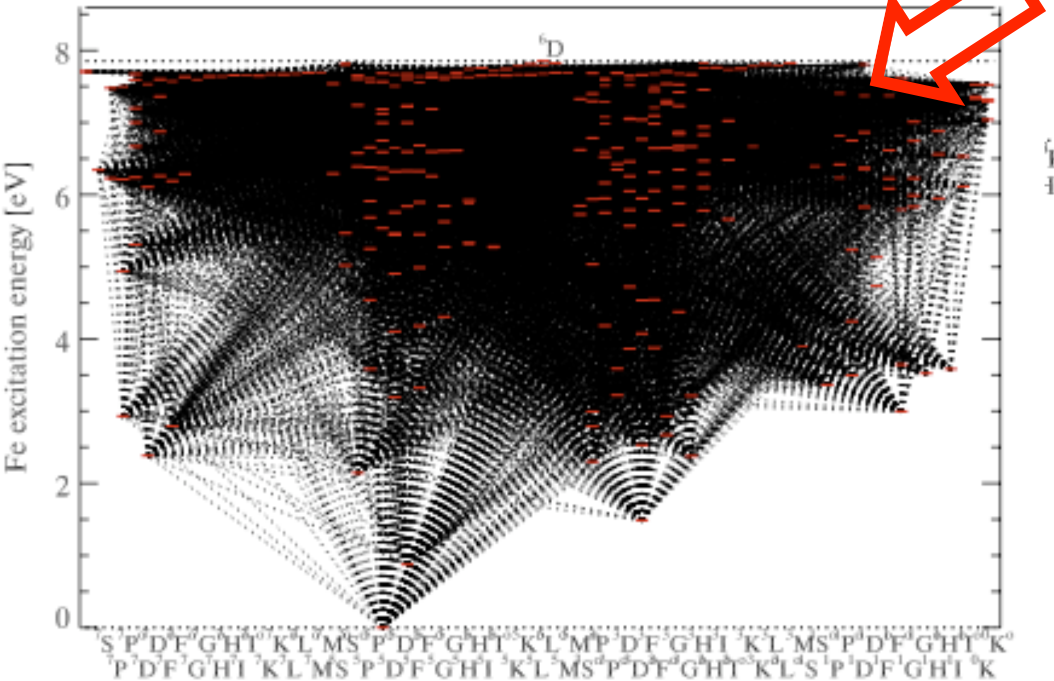
🟨 overrecombination

🟥 resonance line scattering

Heavy elements



Fe I, complete model: ~37 000 levels, ~6 000 000 transitions



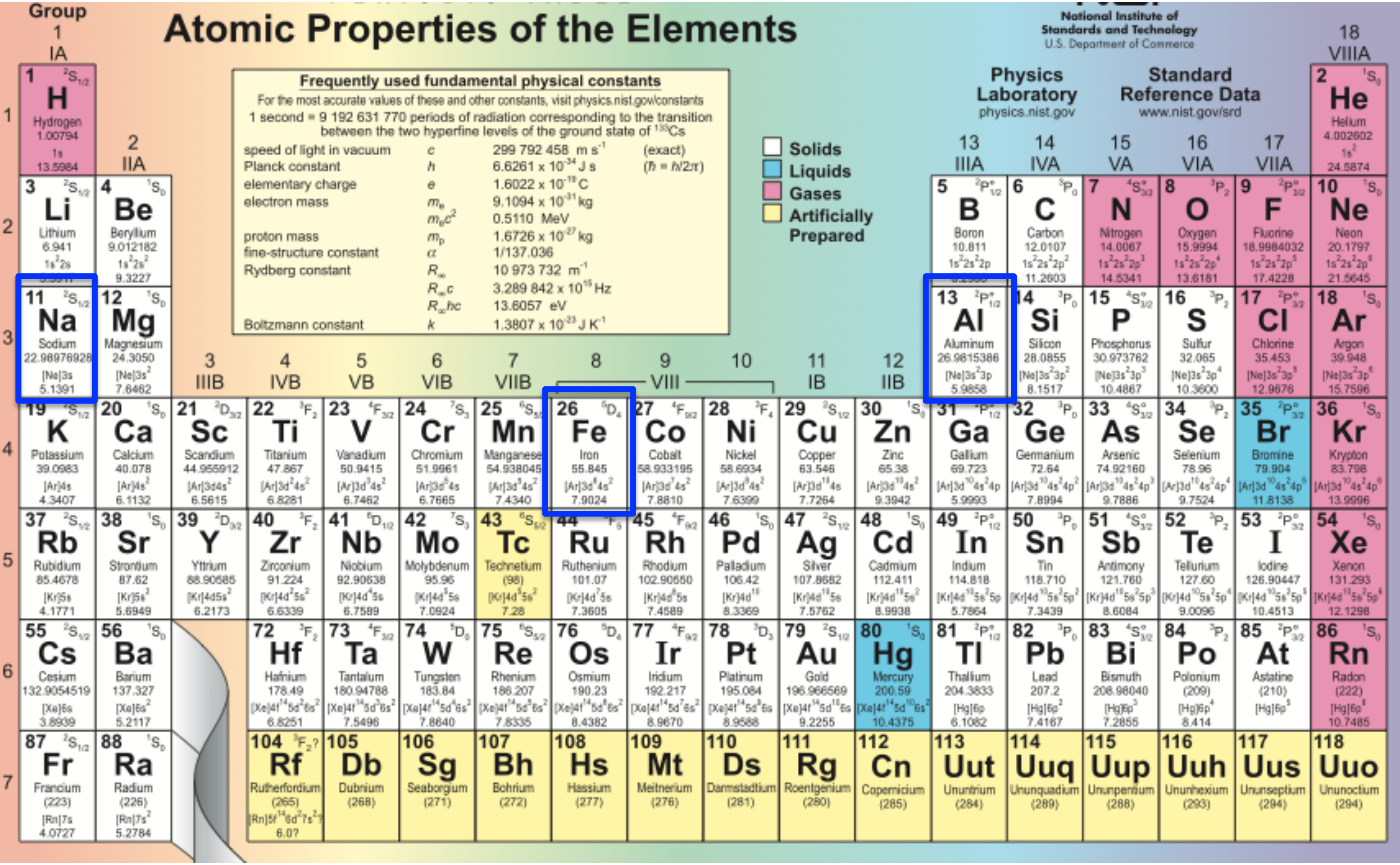
Fe I, reduced model: 300 levels, 13 000 b-b transitions

NLTE: simultaneous solution of RT and SE equations for each ν, i, j:

$$\mu\, dI_\nu/dz = -\alpha I_\nu + \varepsilon$$

$$n_i \sum (C_{ij} + R_{ij}) = \sum n_j (C_{ji} + R_{ji})$$

Bergemann et al. (2012)



Atomic Properties of the Elements

National Institute of Standards and Technology
U.S. Department of Commerce

Physics Laboratory
physics.nist.gov

Standard Reference Data
www.nist.gov/srd

Frequently used fundamental physical constants

For the most accurate values of these and other constants, visit physics.nist.gov/constants

1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs

speed of light in vacuum	c	299 792 458 m s^{-1}	(exact)
Planck constant	h	6.6261 x 10^{-34} J s	($\hbar = h/2\pi$)
elementary charge	e	1.6022 x 10^{-19} C	
electron mass	m_e	9.1094 x 10^{-31} kg	
	m_ec^2	0.5110 MeV	
proton mass	m_p	1.6726 x 10^{-27} kg	
fine-structure constant	α	1/137.036	
Rydberg constant	R_∞	10 973 732 m^{-1}	
	$R_\infty c$	3.289 842 x 10^{15} Hz	
	$R_\infty hc$	13.6057 eV	
Boltzmann constant	k	1.3807 x 10^{-23} J K^{-1}	

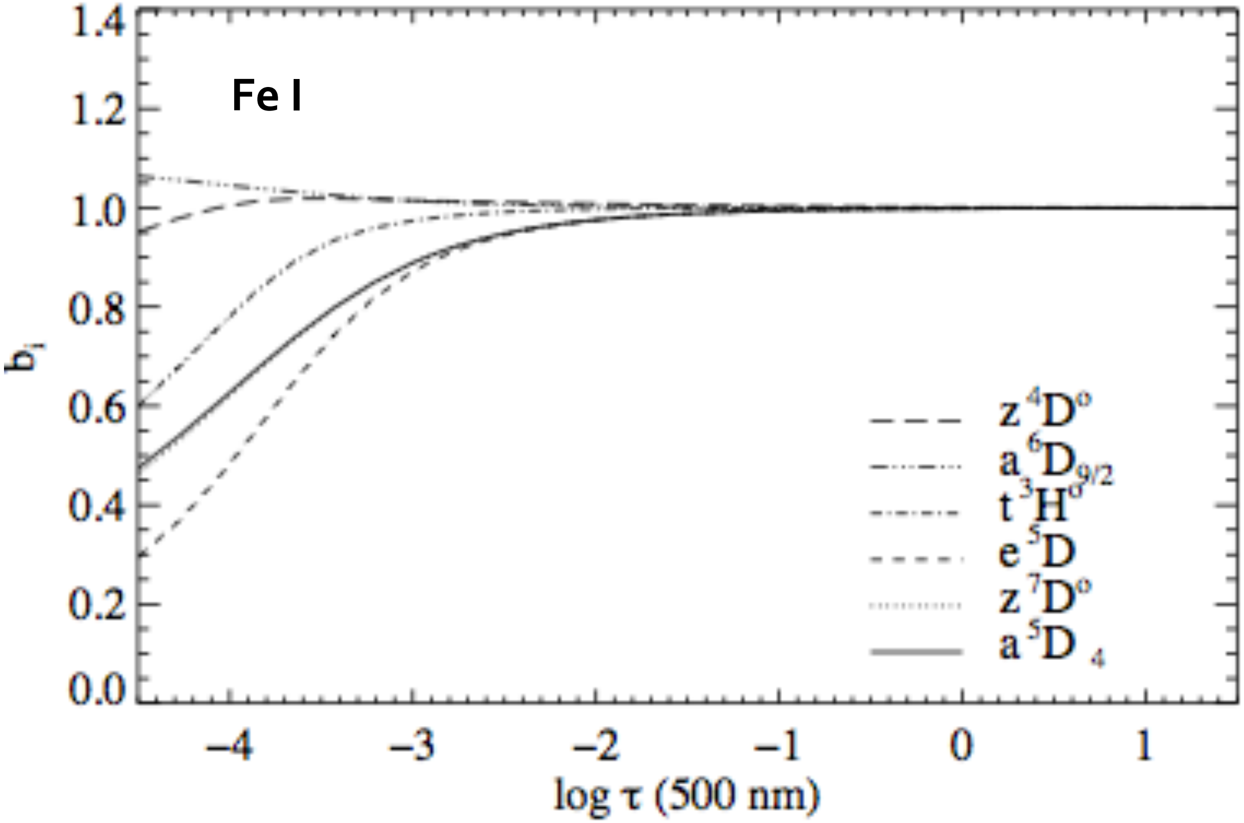
☐ Solids
🟦 Liquids
🟥 Gases
🟨 Artificially Prepared

	Group 1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIII	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 $^2S_{1/2}$ **H** Hydrogen 1.00794 $1s$ 13.5984																	2 $^1S_0$ **He** Helium 4.002602 $1s^2$ 24.5874
2	3 $^2S_{1/2}$ **Li** Lithium 6.941 $1s^22s$	4 $^1S_0$ **Be** Beryllium 9.012182 $1s^22s^2$ 9.3227											5 $^2P^\circ_{1/2}$ **B** Boron 10.811 $1s^22s^22p$	6 $^3P_0$ **C** Carbon 12.0107 $1s^22s^22p^2$ 11.2603	7 $^4S^\circ_{3/2}$ **N** Nitrogen 14.0067 $1s^22s^22p^3$ 14.5341	8 $^3P_2$ **O** Oxygen 15.9994 $1s^22s^22p^4$ 13.6181	9 $^2P^\circ_{3/2}$ **F** Fluorine 18.9984032 $1s^22s^22p^5$ 17.4228	10 $^1S_0$ **Ne** Neon 20.1797 $1s^22s^22p^6$ 21.5645
3	11 $^2S_{1/2}$ **Na** Sodium 22.98976928 [Ne]$3s$ 5.1391	12 $^1S_0$ **Mg** Magnesium 24.3050 [Ne]$3s^2$ 7.6462											13 $^2P^\circ_{1/2}$ **Al** Aluminum 26.9815386 [Ne]$3s^23p$ 5.9858	14 $^3P_0$ **Si** Silicon 28.0855 [Ne]$3s^23p^2$ 8.1517	15 $^4S^\circ_{3/2}$ **P** Phosphorus 30.973762 [Ne]$3s^23p^3$ 10.4867	16 $^3P_2$ **S** Sulfur 32.065 [Ne]$3s^23p^4$ 10.3600	17 $^2P^\circ_{3/2}$ **Cl** Chlorine 35.453 [Ne]$3s^23p^5$ 12.9676	18 $^1S_0$ **Ar** Argon 39.948 [Ne]$3s^23p^6$ 15.7596
4	19 $^2S_{1/2}$ **K** Potassium 39.0983 [Ar]$4s$ 4.3407	20 $^1S_0$ **Ca** Calcium 40.078 [Ar]$4s^2$ 6.1132	21 $^2D_{3/2}$ **Sc** Scandium 44.955912 [Ar]$3d4s^2$ 6.5615	22 $^3F_2$ **Ti** Titanium 47.867 [Ar]$3d^24s^2$ 6.8281	23 $^4F_{3/2}$ **V** Vanadium 50.9415 [Ar]$3d^34s^2$ 6.7462	24 $^7S_3$ **Cr** Chromium 51.9961 [Ar]$3d^54s$ 6.7665	25 $^6S_{5/2}$ **Mn** Manganese 54.938045 [Ar]$3d^54s^2$ 7.4340	26 $^5D_4$ **Fe** Iron 55.845 [Ar]$3d^64s^2$ 7.9024	27 $^4F_{9/2}$ **Co** Cobalt 58.933195 [Ar]$3d^74s^2$ 7.8810	28 $^3F_4$ **Ni** Nickel 58.6934 [Ar]$3d^84s^2$ 7.6399	29 $^2S_{1/2}$ **Cu** Copper 63.546 [Ar]$3d^{10}4s$ 7.7264	30 $^1S_0$ **Zn** Zinc 65.38 [Ar]$3d^{10}4s^2$ 9.3942	31 $^2P^\circ_{1/2}$ **Ga** Gallium 69.723 [Ar]$3d^{10}4s^24p$ 5.9993	32 $^3P_0$ **Ge** Germanium 72.64 [Ar]$3d^{10}4s^24p^2$ 7.8994	33 $^4S^\circ_{3/2}$ **As** Arsenic 74.92160 [Ar]$3d^{10}4s^24p^3$ 9.7886	34 $^3P_2$ **Se** Selenium 78.96 [Ar]$3d^{10}4s^24p^4$ 9.7524	35 $^2P^\circ_{3/2}$ **Br** Bromine 79.904 [Ar]$3d^{10}4s^24p^5$ 11.8138	36 $^1S_0$ **Kr** Krypton 83.798 [Ar]$3d^{10}4s^24p^6$ 13.9996
5	37 $^2S_{1/2}$ **Rb** Rubidium 85.4678 [Kr]$5s$ 4.1771	38 $^1S_0$ **Sr** Strontium 87.62 [Kr]$5s^2$ 5.6949	39 $^2D_{3/2}$ **Y** Yttrium 88.90585 [Kr]$4d5s^2$ 6.2173	40 $^3F_2$ **Zr** Zirconium 91.224 [Kr]$4d^25s^2$ 6.6339	41 $^6D_{1/2}$ **Nb** Niobium 92.90638 [Kr]$4d^45s$ 6.7589	42 $^7S_3$ **Mo** Molybdenum 95.96 [Kr]$4d^55s$ 7.0924	43 $^6S_{5/2}$ **Tc** Technetium (98) [Kr]$4d^55s^2$ 7.28	44 F_5 **Ru** Ruthenium 101.07 [Kr]$4d^75s$ 7.3605	45 $^4F_{9/2}$ **Rh** Rhodium 102.90550 [Kr]$4d^85s$ 7.4589	46 $^1S_0$ **Pd** Palladium 106.42 [Kr]$4d^{10}$ 8.3369	47 $^2S_{1/2}$ **Ag** Silver 107.8682 [Kr]$4d^{10}5s$ 7.5762	48 $^1S_0$ **Cd** Cadmium 112.411 [Kr]$4d^{10}5s^2$ 8.9938	49 $^2P^\circ_{1/2}$ **In** Indium 114.818 [Kr]$4d^{10}5s^25p$ 5.7864	50 $^3P_0$ **Sn** Tin 118.710 [Kr]$4d^{10}5s^25p^2$ 7.3439	51 $^4S^\circ_{3/2}$ **Sb** Antimony 121.760 [Kr]$4d^{10}5s^25p^3$ 8.6084	52 $^3P_2$ **Te** Tellurium 127.60 [Kr]$4d^{10}5s^25p^4$ 9.0096	53 $^2P^\circ_{3/2}$ **I** Iodine 126.90447 [Kr]$4d^{10}5s^25p^5$ 10.4513	54 $^1S_0$ **Xe** Xenon 131.293 [Kr]$4d^{10}5s^25p^6$ 12.1298
6	55 $^2S_{1/2}$ **Cs** Cesium 132.9054519 [Xe]$6s$ 3.8939	56 $^1S_0$ **Ba** Barium 137.327 [Xe]$6s^2$ 5.2117		72 $^3F_2$ **Hf** Hafnium 178.49 [Xe]$4f^{14}5d^26s^2$ 6.8251	73 $^4F_{3/2}$ **Ta** Tantalum 180.94788 [Xe]$4f^{14}5d^36s^2$ 7.5496	74 $^5D_0$ **W** Tungsten 183.84 [Xe]$4f^{14}5d^46s^2$ 7.8640	75 $^6S_{5/2}$ **Re** Rhenium 186.207 [Xe]$4f^{14}5d^56s^2$ 7.8335	76 $^5D_4$ **Os** Osmium 190.23 [Xe]$4f^{14}5d^66s^2$ 8.4382	77 $^4F_{9/2}$ **Ir** Iridium 192.217 [Xe]$4f^{14}5d^76s^2$ 8.9670	78 $^3D_3$ **Pt** Platinum 195.084 [Xe]$4f^{14}5d^96s$ 8.9588	79 $^2S_{1/2}$ **Au** Gold 196.966569 [Xe]$4f^{14}5d^{10}6s$ 9.2255	80 $^1S_0$ **Hg** Mercury 200.59 [Xe]$4f^{14}5d^{10}6s^2$ 10.4375	81 $^2P^\circ_{1/2}$ **Tl** Thallium 204.3833 [Hg]$6p$ 6.1082	82 $^3P_0$ **Pb** Lead 207.2 [Hg]$6p^2$ 7.4167	83 $^4S^\circ_{3/2}$ **Bi** Bismuth 208.98040 [Hg]$6p^3$ 7.2855	84 $^3P_2$ **Po** Polonium (209) [Hg]$6p^4$ 8.414	85 $^2P^\circ_{3/2}$ **At** Astatine (210) [Hg]$6p^5$	86 $^1S_0$ **Rn** Radon (222) [Hg]$6p^6$ 10.7485
7	87 $^2S_{1/2}$ **Fr** Francium (223) [Rn]$7s$ 4.0727	88 $^1S_0$ **Ra** Radium (226) [Rn]$7s^2$ 5.2784		104 $^3F_2$? **Rf** Rutherfordium (265) [Rn]$5f^{14}6d^27s^2$? 6.0?	105 **Db** Dubnium (268)	106 **Sg** Seaborgium (271)	107 **Bh** Bohrium (272)	108 **Hs** Hassium (277)	109 **Mt** Meitnerium (276)	110 **Ds** Darmstadtium (281)	111 **Rg** Roentgenium (280)	112 **Cn** Copernicium (285)	113 **Uut** Ununtrium (284)	114 **Uuq** Ununquadium (289)	115 **Uup** Ununpentium (288)	116 **Uuh** Ununhexium (293)	117 **Uus** Ununseptium (294)	118 **Uuo** Ununoctium (294)

Examples: Fe I

$b_m = n_m$ (NLTE)/ n_m (LTE)

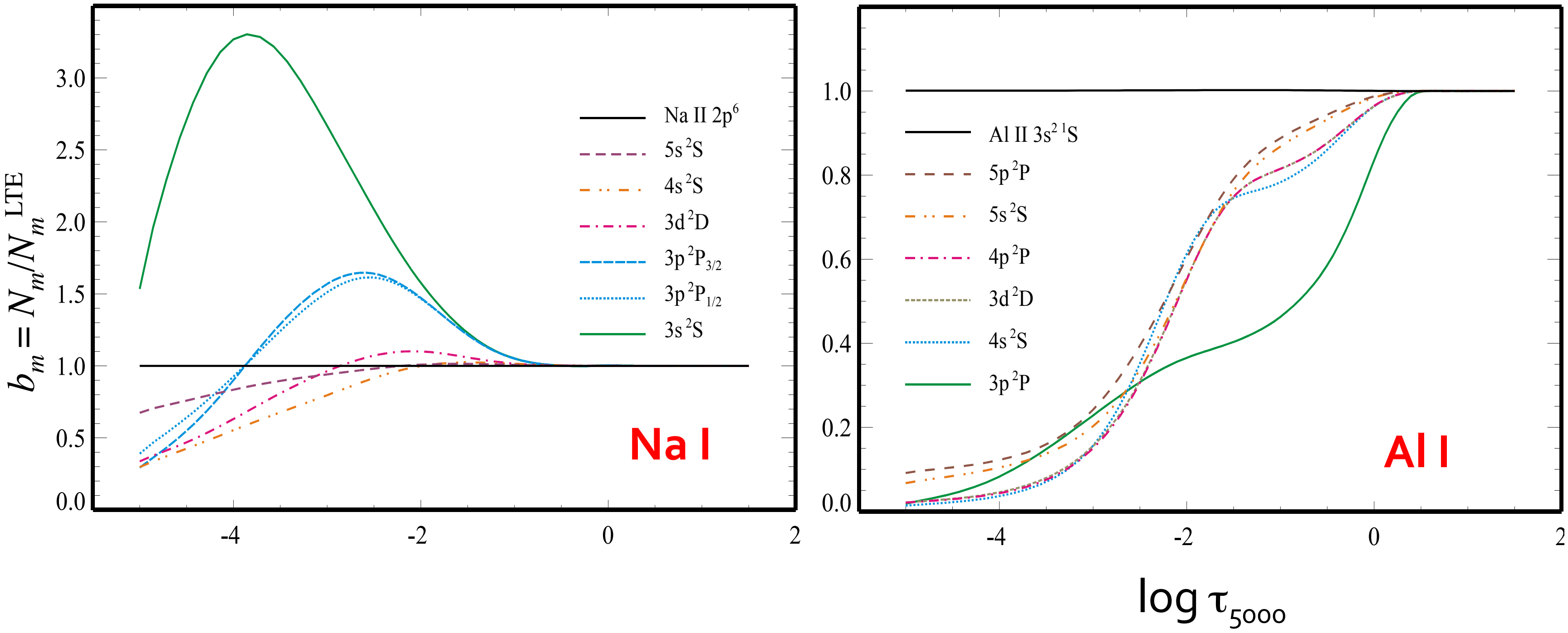
- $J_\nu > B_\nu(T_{local})$ in the UV   over-ionization from the low-excited levels



Bergemann et al. (2012)

Examples: Na I, Al I

- $J_\nu > B_\nu(T_{local})$ in the UV   over-ionization from the low-excited levels
- $J_\nu < B_\nu(T_{local})$ in the IR   over-recombination to the high-excited levels

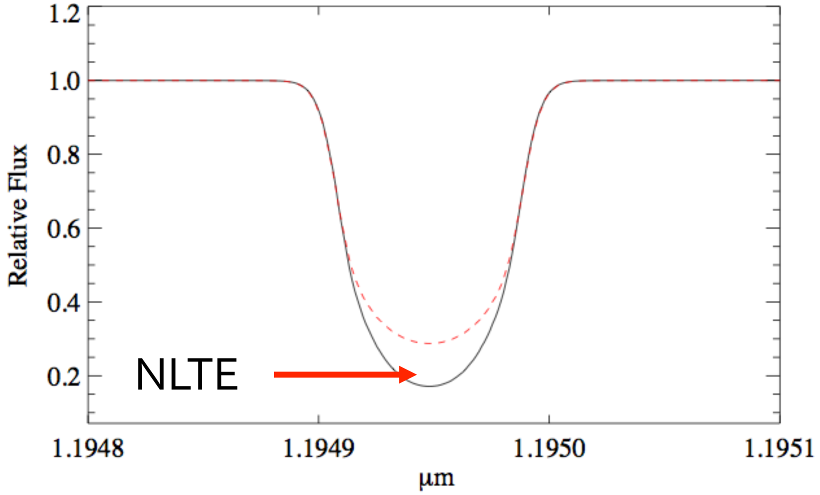


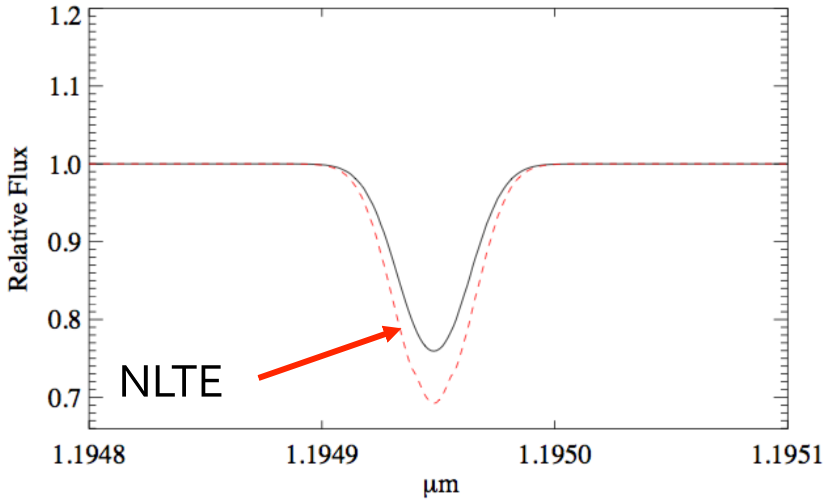
NLTE effects on line profiles

changes in the line opacity k_n (~ τ) and line source function S

$$I_\nu = \int_0^\infty S_\nu e^{-\tau_\nu} d\tau_\nu$$

as a result, line strengthening or weakening, or both





Change of line opacity k_n and line source function S_n determine strength and shape of a spectral line:

$$I_\nu = \int_0^\infty S_\nu e^{-\tau_\nu} d\tau_\nu$$

$k_n \sim b_i$

$S_n \sim B_n b_j/b_i$

if $b_i < 1$, then $k_{NLTE} < k_{,LTE}$

NLTE line weaker than in LTE

if $b_i > b_j$, then $S_n < B_n b_j/b_i$

NLTE line stronger than in LTE