Processes and Diagnostics in Collisional Plasmas

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AtomDB Workshop, Tokyo Metropolitan University
September 2014

(*) standing on the shoulders of many others references:

1. S. M. Kahn: *Soft X-ray spectroscopy of Astrophysical Plasmas*, High-energy Spectroscopic Astrophysics, Saas-Fee Advanced Course **30**, 2000, Les Diablerets, Switzerland

2. Jelle Kaastra *et al.*, *Thermal Radiation Processes*, Space Sci. Rev., **134**, 155 (2008)

collisional processes

photons emitted in transitions i > j:

quantum mechanical calculation requires:

atomic structure model

transition probabilities

plasma/spectral modeling requires:

rate equations

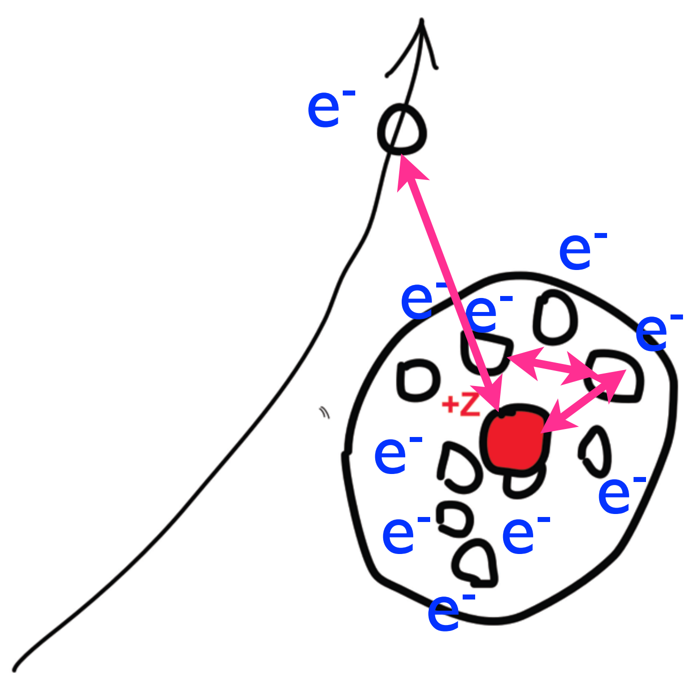
astrophysics requires:

diagnostics

and each of these involves approximations!

collisional processes

atomic excitation by collision ('impact') with charged particle (e^-, p, ion, e^+, even atom, ...): kinetic energy projectile → photon energy

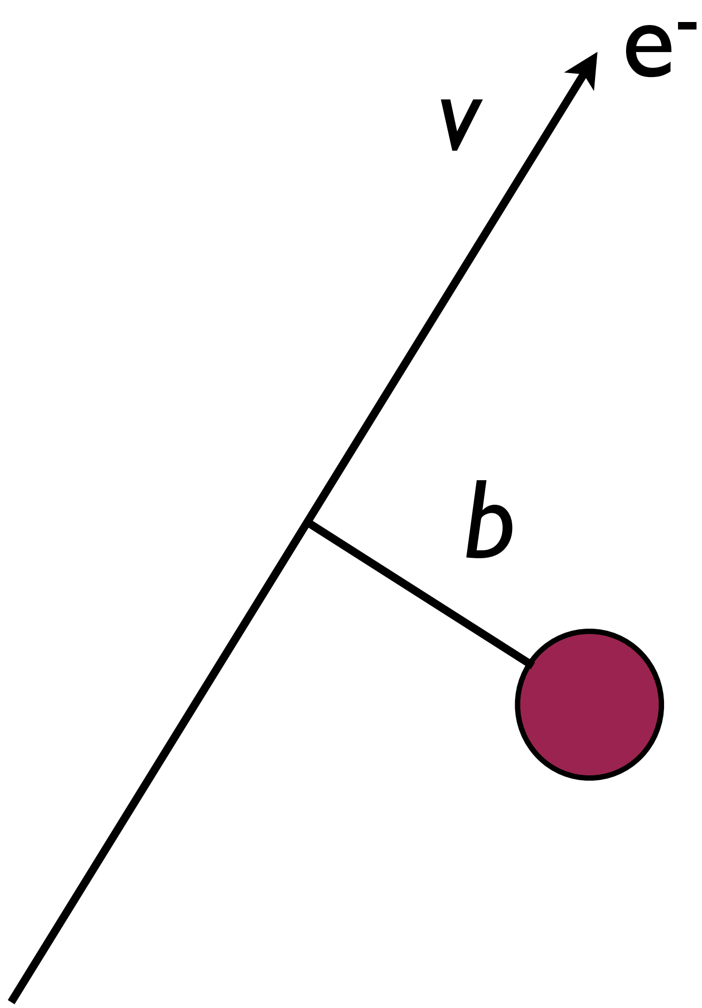


Coulomb force

also: spins interact with currents, etc.!

complex problem!
write Schroedinger equation (Dirac equation) for all the charges (projectile+ion), solve; compute excitation probabilities...

simple classical estimate:



Coulomb force between passing and bound electron:

$$\Delta p = \int F dt \sim \frac{e^2}{b^2} \times \frac{2b}{v} \;\Rightarrow$$

$$\Rightarrow \Delta E = \frac{(\Delta p)^2}{2m} = \frac{2e^4}{mb^2v^2} \equiv E_{ij}$$

cross section: $\sigma_{ij} \sim \pi b^2 = \frac{2\pi e^4}{mv^2 E_{ij}}$

traditional: define *collision strength*, Ω_{ij}:

$$\sigma_{ij} = \frac{\pi a_0^2}{g_i(mv^2)}\Omega_{ij}; \quad \Omega_{ij}(\text{classical}) \ = \frac{4g_i}{E_{ij}}$$

(almost independent of projectile energy)

thermal excitation rate (electron impact):

$$\text{excitations per unit volume per sec} =$$

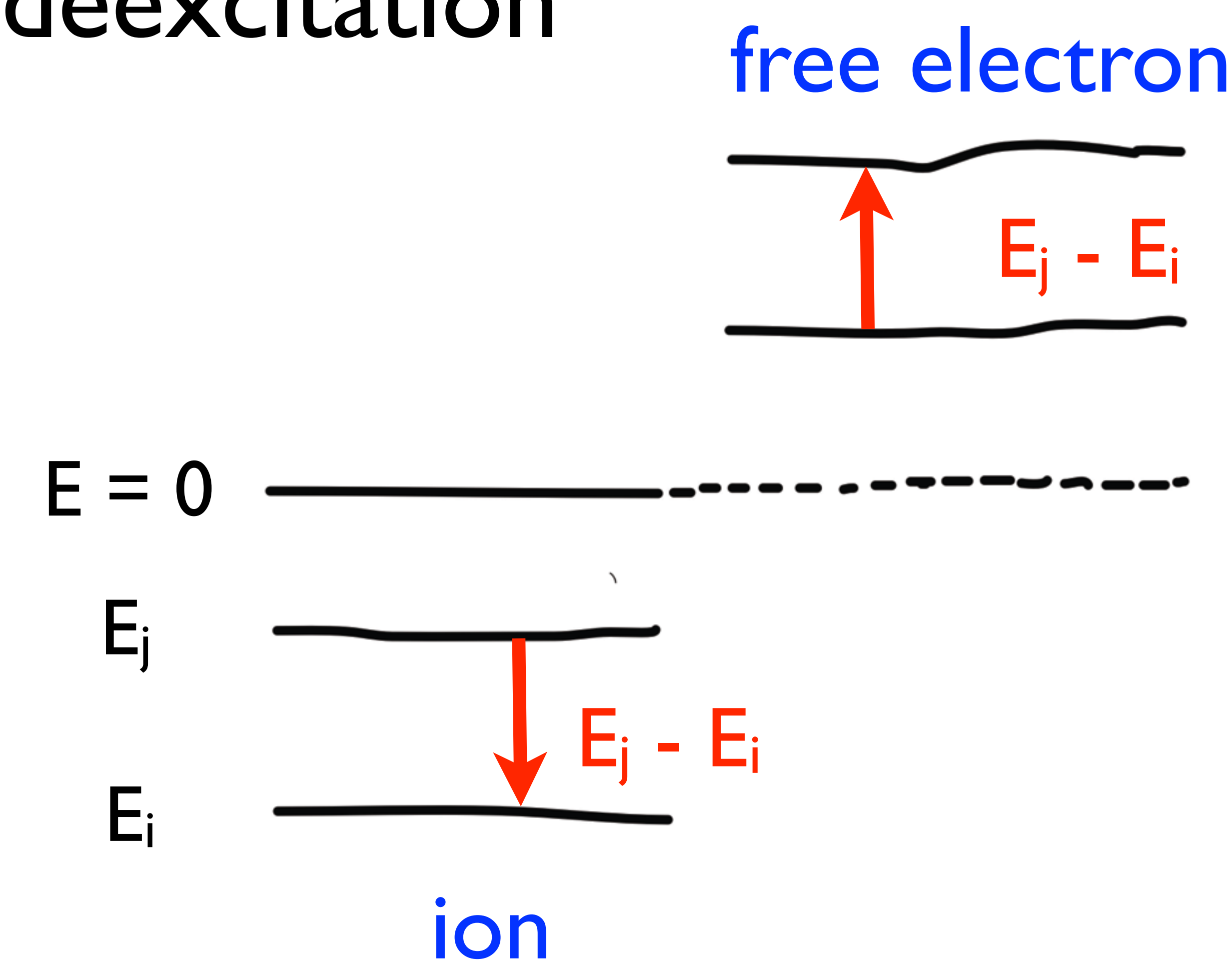
$$= \langle n_e n_i \sigma_{ij} v \rangle \equiv n_e n_i C_{ij}(T);$$

$$C_{ij}(T) \approx \frac{8.6 \times 10^{-6}}{g_i} \ \Omega_{ij} T^{-1/2} \exp(-E_{ij}/kT) \ \text{cm}^3 \ \text{sec}$$

a_0: Bohr radius

and similar calculations for (the) other collisional processes:

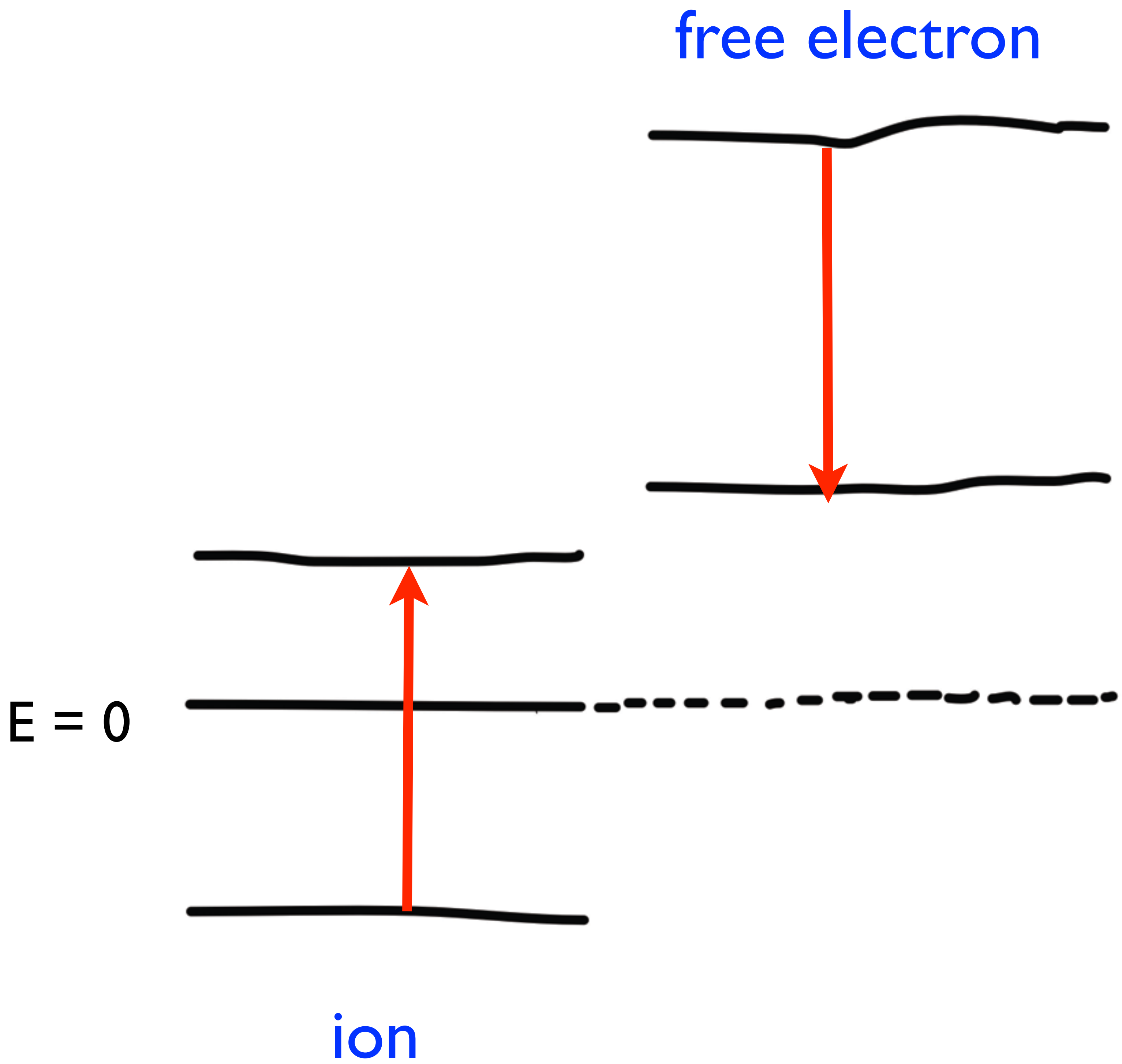
inverse of collisional excitation:
collisional deexcitation



note: get all rates for inverse processes from detailed balance in thermodynamic equilibrium (so $n_i/n_j = g_i/g_j \exp(-E_{ij}/kT)$)

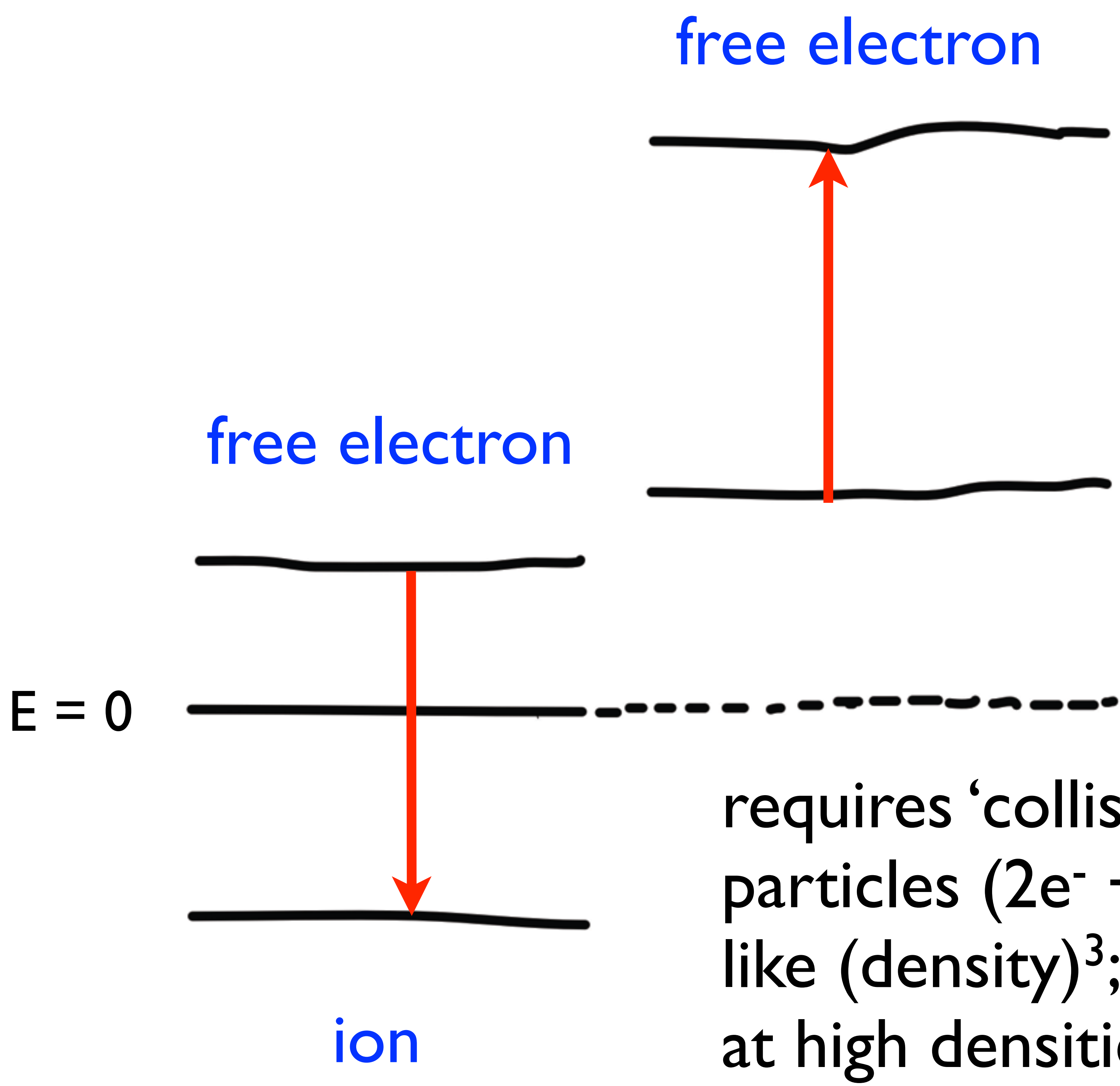
other collisional processes

collisional ionization



other collisional processes

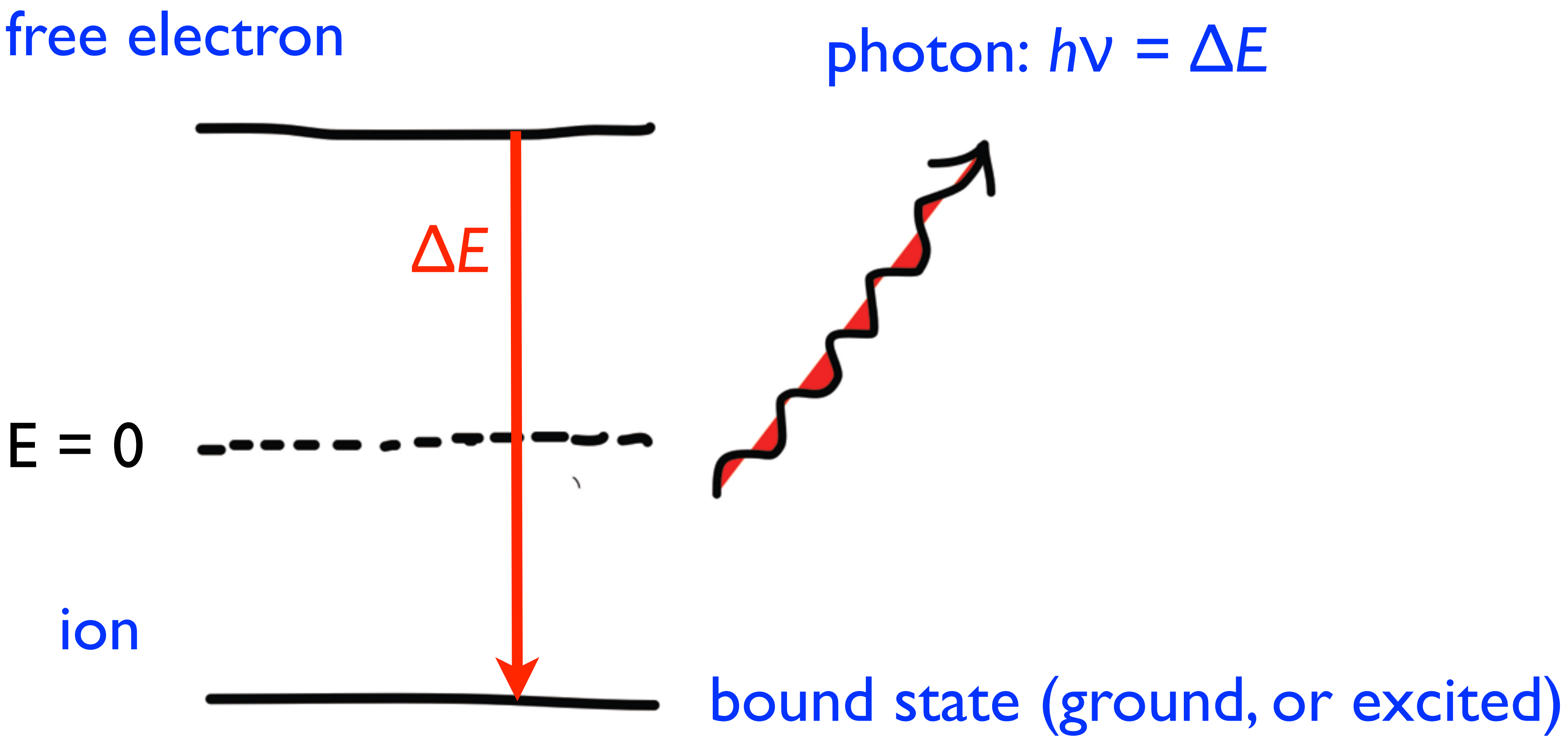
inverse of collisional ionization:
3-body recombination



requires 'collision' of three particles ($2e^- + i$), so goes like (density)^3; only important at high densities

other collisional processes

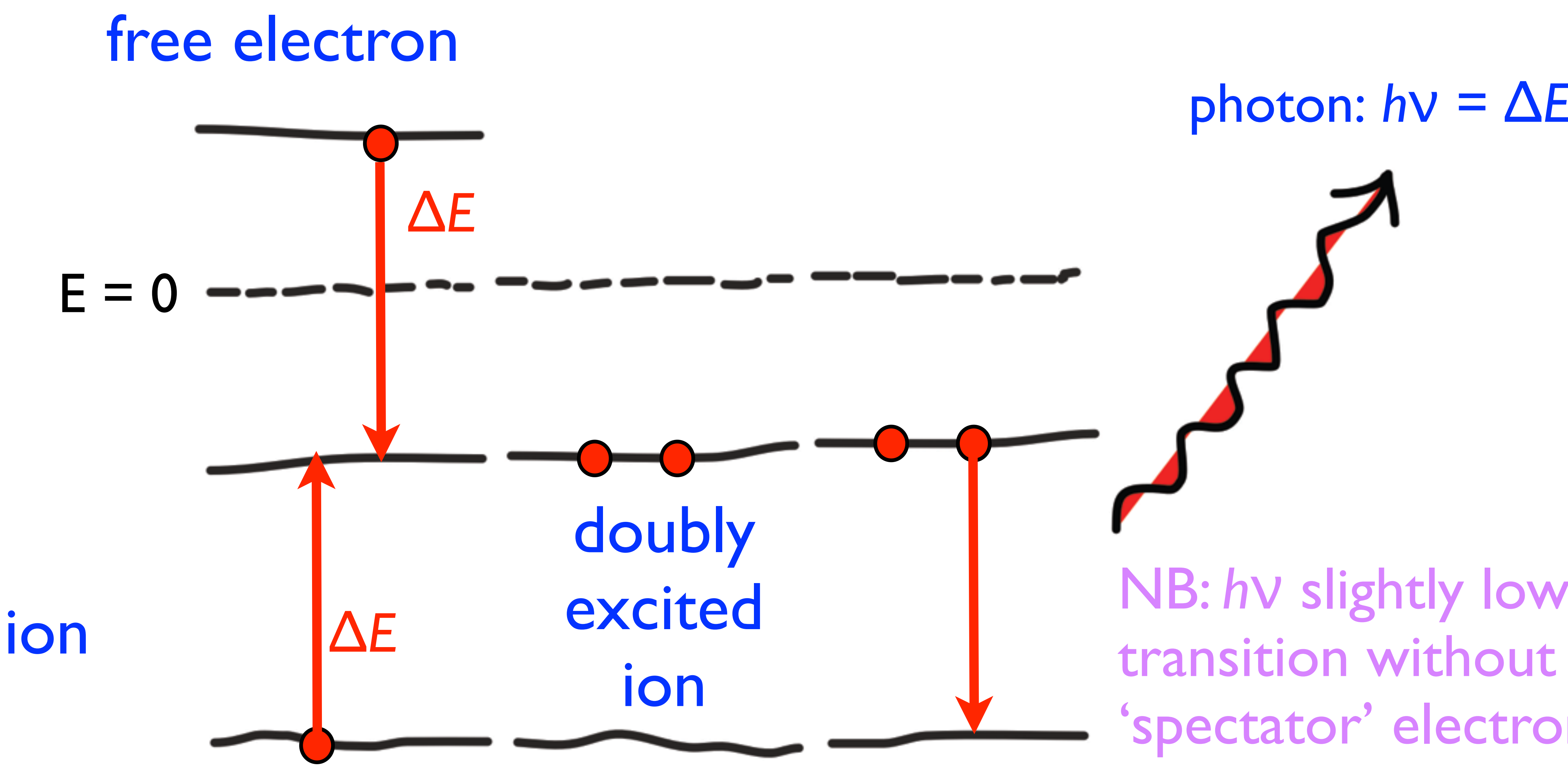
radiative recombination (inverse of photoionization)



other collisional processes

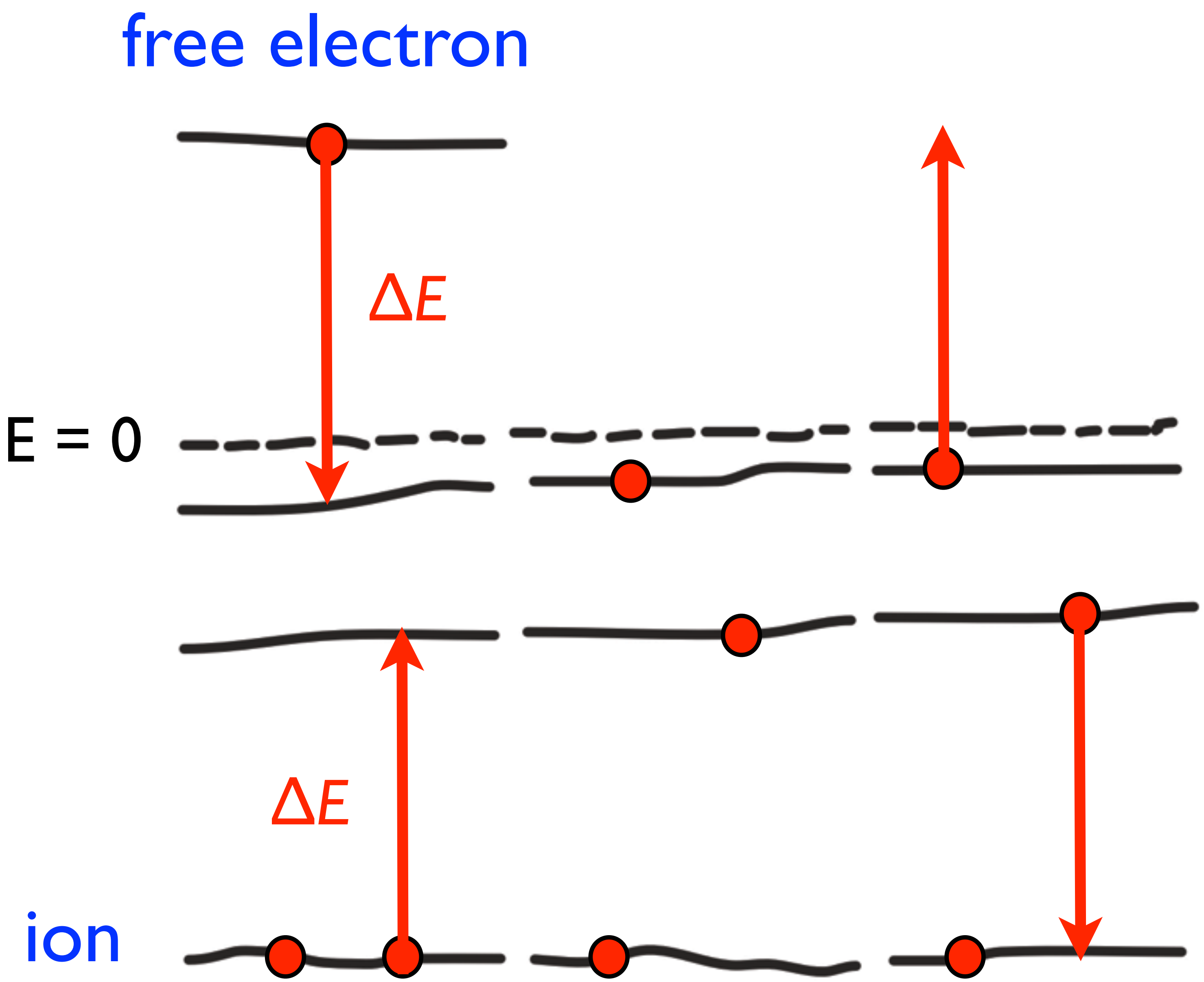
dielectronic recombination

NB: ΔE has to be fairly large: need enough energy to excite e^- from ground



NB: $h\nu$ slightly lower than transition without second ‘spectator’ electron: ‘parent’ and ‘satellite’ lines

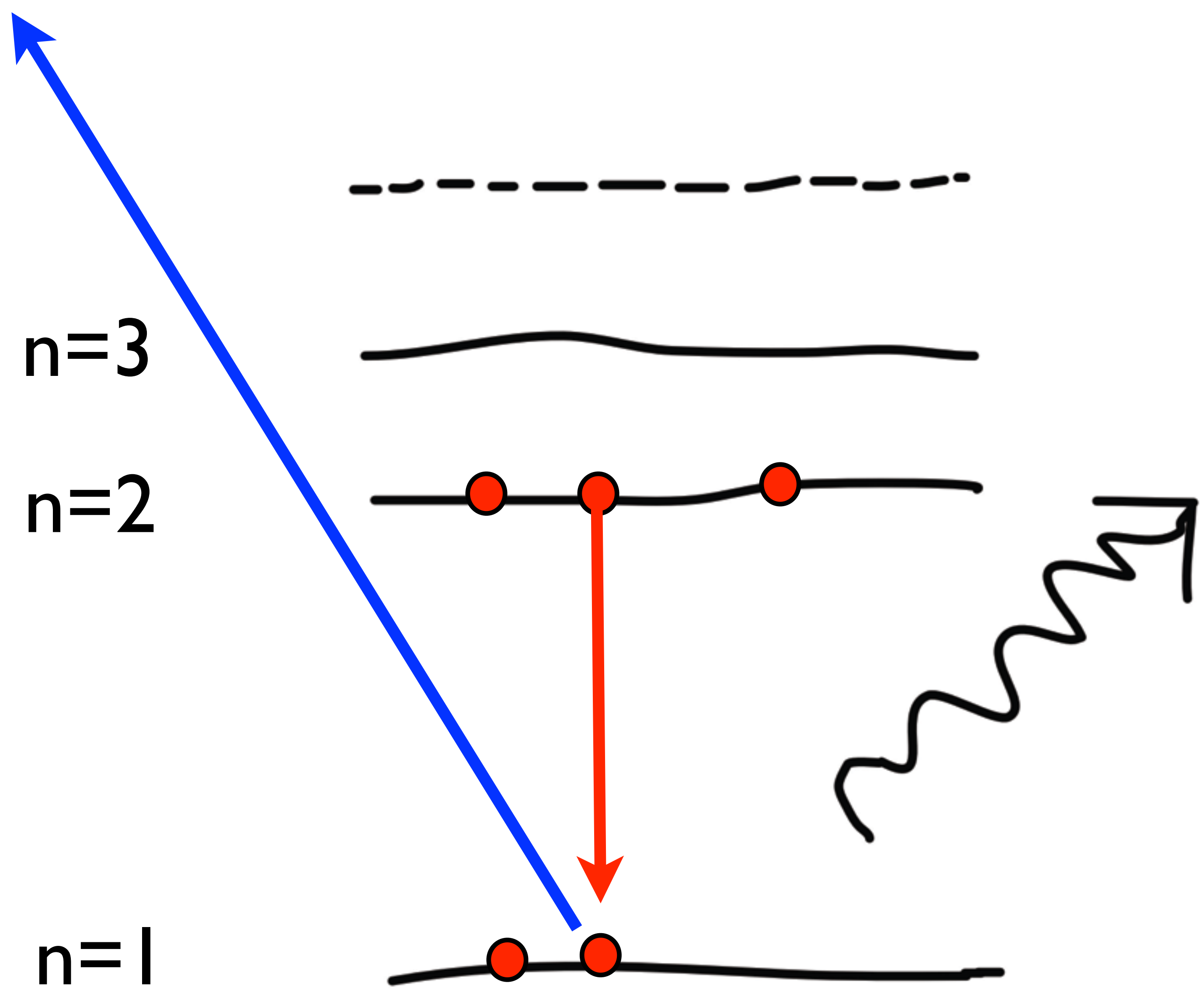
dielectronic recombination:
alternative outcome: autoionization (Auger)



NB: in complex ions, autoionization more likely than radiative decay.
Can also lead to emission of *several* electrons in same decay!

other collisional processes

in more complex ions: ‘innershell’ processes
(in neutral atoms, usually called ‘fluorescence’)



especially important in ionizing plasmas!

other collisional processes

other projectiles:
protons, ions, positrons...

of these, protons (usually) the most abundant,
so proton impact excitation could be important

but:

naive classical argument suggests: $\sigma \sim (mv^2)^{-1}$,
and in kinetic equilibrium, $\langle m_e v_e^2 \rangle = \langle m_p v_p^2 \rangle$,
so the rate $\langle n_p n_i \sigma v_p \rangle$ is low because v_p is low

other collisional processes

what else collisional?

charge exchange

subject of Randall's talk

collisions with non-thermal/cosmic ray particles

same principles, different rates (no T)

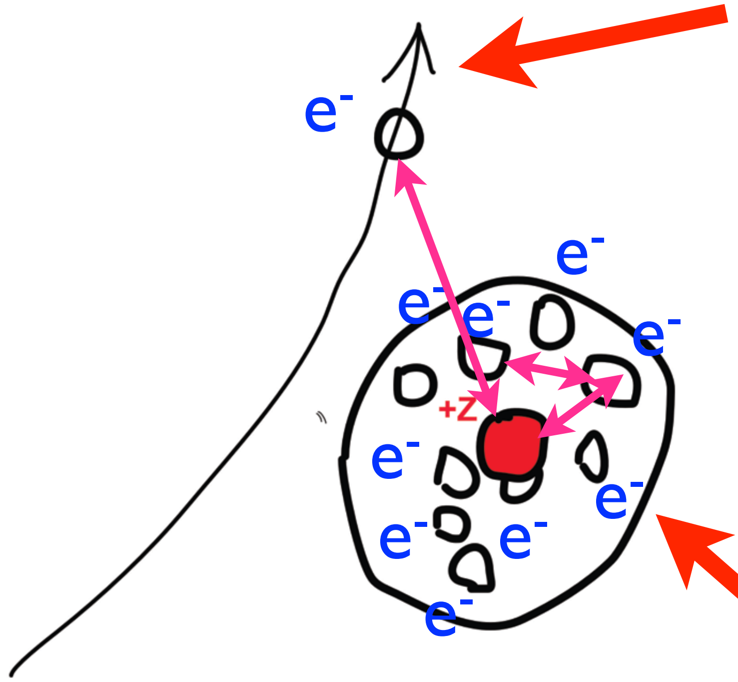
quantum theory of collisions (outline)

general problem:
write Hamiltonian for entire system, solve for given initial state, find probability of given final state...(*)

in practice, make series of (independent) approximations

(*) ignoring extreme relativity, QED

approximations



1. fix the trajectory of the projectile

special case: initial and final state of projectile: free particle (‘Born approximation’). Better: use solutions to Schroedinger Equation for free particle in real atomic potential (‘distorted wave’)

2. assume the interaction does not change the structure of the ion

ion structure can be calculated separately; collision only causes transitions between states

3. effect of collision interaction is weak/slow: apply (time-dependent) perturbation theory

electron collisions:
total wavefunctions for initial and final states have to be completely antisymmetric under interchange of **any** two electrons!
(so that includes the projectile!
you have to consider the possibility of incoming and bound electron changing places!)

(Inelastic) Scattering Theory

CC, R-matrix, CCC, ...

incident electron

N bound electrons

$$i\hbar \frac{\partial \Psi(\mathbf{r}_0; \mathbf{r}_1, ..., \mathbf{r}_N, t)}{\partial t} = H\Psi(\mathbf{r}_0; \mathbf{r}_1, ..., \mathbf{r}_N, t);$$

$$H = -\frac{\hbar^2}{2m}(\nabla_0^2 + \nabla_1^2 + ... + \nabla_N^2) + V(\mathbf{r}_0; \mathbf{r}_1, ..., \mathbf{r}_N)$$

Coulomb force, **all** electrons with nucleus, and with each other

NB: nonrelativistic, no spin; but can also do this with a 'Dirac Hamiltonian'

Now seek stationary solution that represents constant flux of incident and scattered particles:

total kinetic + potential energy

$$\Psi(\mathbf{r}_0; \mathbf{r}_1, ..., \mathbf{r}_N, t) = \psi(\mathbf{r}_0; \mathbf{r}_1, ..., \mathbf{r}_N) \exp(-iEt/\hbar)$$

and represent the total wavefunction for the bound electrons with the eigenstates of the unperturbed target, times a wavefunction for the incident/scattered electron

example with two electrons (e^- colliding with H-like ion):

bound electron

$$\psi^{\pm}(\mathbf{r}_0, \mathbf{r}_1) \rightarrow_{r_0 \rightarrow \infty} \sum_j F_j^{\pm}(\mathbf{r}_0)\psi_j(\mathbf{r}_1) \pm F_j^{\pm}(\mathbf{r}_1)\psi_j(\mathbf{r}_0)$$

incident electron

far away from atom

all bound states than can be excited (enough KE)

try this for the scattered particle:

$$F_j^{\pm}(\mathbf{r}) \rightarrow_{r \rightarrow \infty} \underbrace{\exp(i\mathbf{k}_i \cdot \mathbf{r})\delta_{ij}}_{\text{in}} + \underbrace{f_{ji}^{\pm}(k_i, \theta, \phi)\frac{e^{ik_j r}}{r}}_{\text{out}}$$

and insert into Schroedinger equation;
make approximations for the sum over states
from the solutions, get the scattering amplitudes f_{ij};
from the scattering amplitudes, get the cross section

Approximate Solutions

1. 'Close Coupling'

In the expression for $\psi(\boldsymbol{r}_0,\boldsymbol{r}_1)$, keep *finite* set of states ψ_j
The Schroedinger equation becomes a set of coupled integro-differential equations for the F_j in terms of the known ψ_j ; solve numerically.

2. 'R-matrix'

divide the range of *r* into 'near' and 'far'

near	*far*
N+1 electrons; resembles bound system	asymptotically: ion + free electron (Ψ simple)
r < a	r > a

r = a

match solutions on r=a

3. Convergent Close Coupling ('CCC')

In the expansion for $\psi(\boldsymbol{r}_0,\boldsymbol{r}_1)$, include not just the bound 'target states' $\psi_j(\boldsymbol{r})$, but also the continuum states; with sufficient computing power, *calculation for the cross sections converges...*
and is generally in very good agreement with experiments.

It is instructive to look at collisions with particles at energies large compared to the excitation energy:
incoming/outgoing electron plane wave; transfer of E and $\boldsymbol{p}$ small ("Born approximation")

can apply t-dependent perturbation theory

Perturbation Theory

time-dependent Schroedinger Equation:
H gives time evolution of wave function.

$$H\left|\psi\right\rangle = i\hbar\frac{\partial\left|\psi\right\rangle}{\partial t}$$

Assume *H* has small part, H^1, that describes the interaction of projectile with target ion; H^0 describes unperturbed ion:

$$H = H^0 + H^1; \quad H^1 \ll H^0; \quad H_0\left|n\right\rangle = E_n\left|n\right\rangle$$

expand ψ on the eigenstates $|n>$ of H^0,

$$\left|\psi(t)\right\rangle = \sum_n a_n(t)\left|n\right\rangle e^{-iE_n t/\hbar}$$

and substitute in Schroedinger Equation, find equation for the $a_n(t)$:
gives the probability that the system is in given state after time *t*, for given initial state, due to perturbation.

transition probability n → m is proportional to $\left| \langle m \left| H^1 \right| n \rangle \right|^2$

two important cases:

vector potential for EM field (*usually plane waves*)

(weak) radiation: $$H^1 = -\frac{ie\hbar}{mc} \left(\mathbf{A} \cdot \nabla \right)$$

electron coordinates

charged particle: $$H^1 = \frac{e^2}{\left| \mathbf{r}_1 - \mathbf{r}_2 \right|}$$

electron coordinates

coordinates of perturber (assumed e^-)

‘selection rules’:

weak radiation: *plane wave*

look at $\langle \mathrm{final} \,|\, H^1 \,|\, \mathrm{initial} \rangle$

charged particle in Born Approximation: *plane wave*

$$\exp(-i\mathbf{k}\cdot\mathbf{r}) \rightarrow 1 - i\mathbf{k}\cdot\mathbf{r} - \frac{1}{2}(\mathbf{k}\cdot\mathbf{r})^2 + \ldots \quad (\mathbf{k}\cdot\mathbf{r} \ll 1)$$

Gives rise to ‘selection rules’.

Dipole approximation: keep the 1; if matrix element is zero, next order transition probability is ~ $(\boldsymbol{k}.\boldsymbol{r})^2$ ~ $(v/c)^2$ ~ $(Z\alpha)^2$ times smaller!

selection rules for radiative and collisional processes are similar (to lowest approximation)!

Atomic Structure, Multielectron Systems

atomic energy budget:

1. kinetic energy; Coulomb potential nucleus
2. Coulomb repulsion e^--e^-
3. spin (magnetic moment) with currents ("$\boldsymbol{L}.\boldsymbol{S}$")
4. small: spin-spin; electron spin-nuclear spin;
   relativity; QED

focus on 1,2, and use the NR Schroedinger Equation;
3 and 4: can be added as perturbations (or [3], use Dirac equation from the start)

Atomic Structure

Approximation: Central Field

electrons see:

$V_{\text{nucleus}}(r)$

$V_{\text{other electrons}}(r)$ } *spherically symmetric*

residual $V_{ee}(r_{12})$ *not sph. symmetric*

V(r) determines atomic structure, but depends on the solution! (nonlinear problem)

Try solutions built up from products of one-electron ‘orbitals’, completely antisymmetric (‘Slater Determinant’);
perturbation theory to find best solution → Hartree-Fock equations, get Ψ and *V(r)*; iterate

There is spin-dependence even though H spin-independent! because of requirement of complete antisymmetry (*both* in $\boldsymbol{r}_i$ *and* spins!)

example with 2 electrons:

write solutions as products $\varphi(\boldsymbol{r}_1,\boldsymbol{r}_2)\ \chi(\text{spin } 1, \text{spin } 2)$;
has to be asymmetric under $\boldsymbol{r}_1 \rightleftarrows \boldsymbol{r}_2$ or $s_1 \rightleftarrows s_2$

if χ symmetric, φ must be antisymmetric, and v.v.

possible solutions for χ (*i.e.* stationary states, constant total spin):

$\uparrow\uparrow$

$\downarrow\downarrow$

$\uparrow\downarrow + \downarrow\uparrow$

symmetric, spin 1

$\uparrow\downarrow - \downarrow\uparrow$

antisymmetric, spin 0

multielectron configurations: quick reminder of L-S scheme

if interaction of spins with currents ('***L.S***') is small compared to Coulomb energies, solutions can be written in terms of states of definite total ***L*** and ***S***
(each $\boldsymbol{L}_i$ and $\boldsymbol{S}_i$ conserved, so ***L*** and ***S*** conserved)

spatial wavefunction x spin wavefunction:
(orbital 1)(orbital 2)..... $^{2S+1}L_J$

so e.g. ground state two electron system: $1s^2\ {}^1S_0$

symmetric, $L = 0$

must be antisymmetric, $S = 0$

codes/packages:

HULLAC
(Hebrew University Lawrence Livermore Atomic Code):
Bar-Shalom, Klapisch, & Oreg, Phys Rev A, **38**, 1773 (1988)
(and many updates and improvements)

FAC ("Flexible Atomic Code"): Mingfeng Gu
Can J Phys **86**, 675 (2008)

Rates

Thermal Plasmas: free particle KE distribution Maxwellian. Given all cross sections for collisional excitation, deexcitation, ionization, recombination as a function of projectile kinetic energy: average over $f(v)$, get *rate coefficients* $C_{ij}(T)$ as a function of T.

Definition:

nr of transitions $i \rightarrow j$ per second per unit volume =

$n_e n_i C_{ij}(T)$;

dimension of C_{ij}: $cm^3\ sec^{-1}$

Rate Equations

$$\frac{dn_i}{dt} = +\{\text{all processes into } i\} - \{\text{all processes out of } i\}$$

$$= R_{ij} n_j$$

(if electron collisions only):

$$= n_e C_{ij} n_j$$

equilibrium: $$\frac{dn_i}{dt} = 0$$

Ionization Equilibrium

ignore radiative processes;
rate coefficients only depend on *T*, not *n*;
solve $R_{ij}n_j = 0$; solution $n_j(T)$ depends only on *T*: "***CIE***"

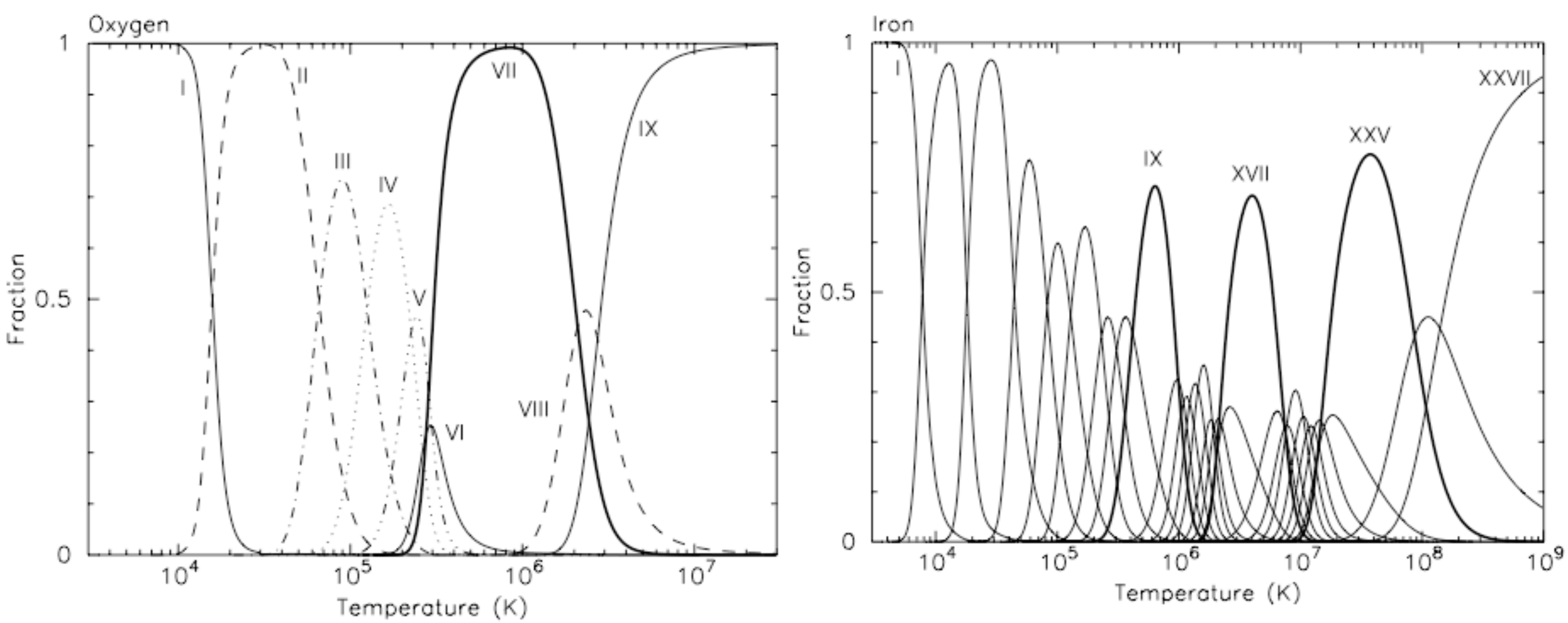
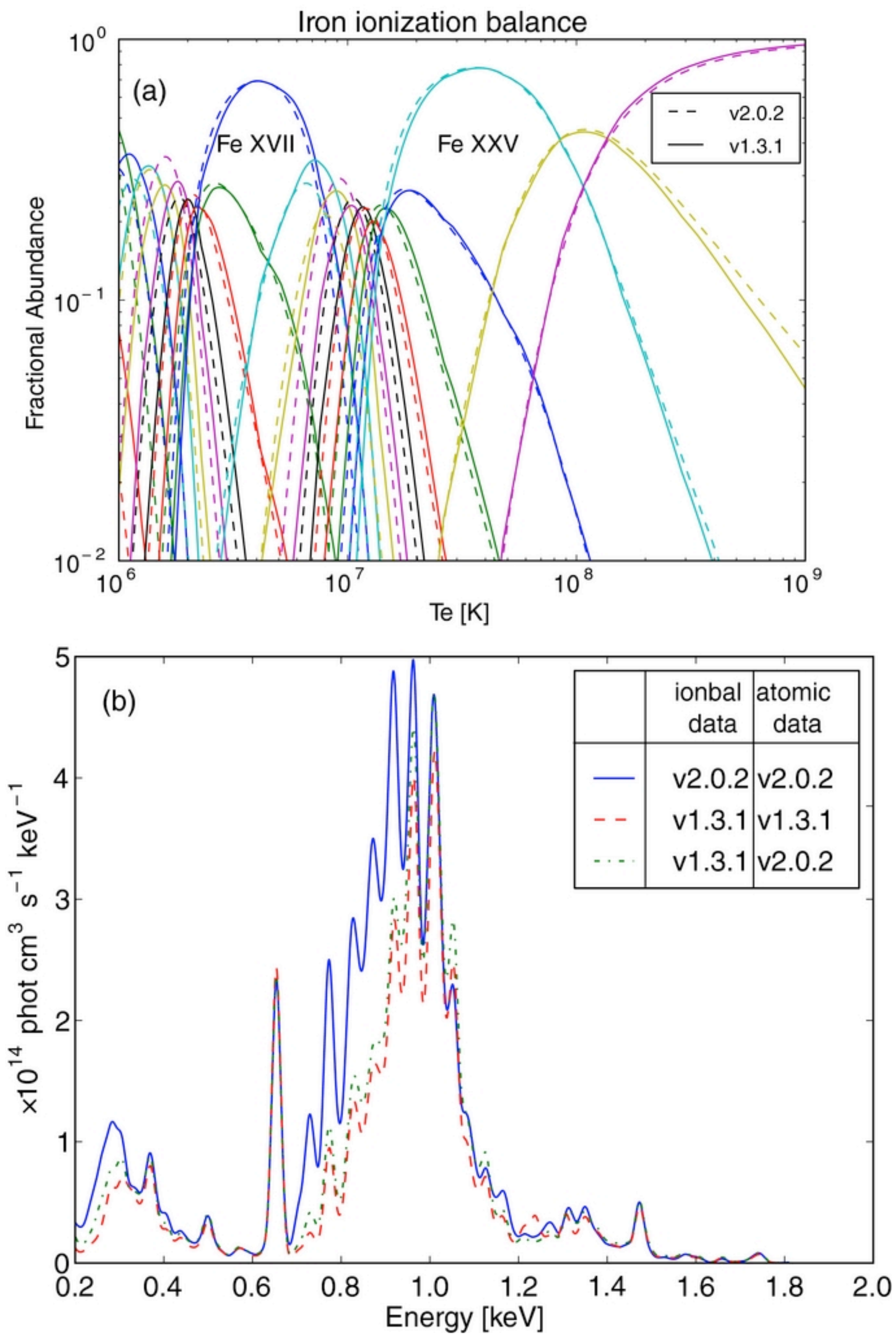


Fig. 7 Ion concentration of oxygen ions (*left panel*) and iron ions (*right panel*) as a function of temperature in a plasma in Collisional Ionisation Equilibrium (CIE). Ions with completely filled shells are indicated with *thick lines*: the He-like ions O VII and Fe XXV, the Ne-like Fe XVII and the Ar-like Fe IX; note that these ions are more prominent than their neighbours

Kaastra *et al.* (2008)

Ionization Equilibrium



K shell ions: relatively simple
L shell ions:
Fe L very important, complex

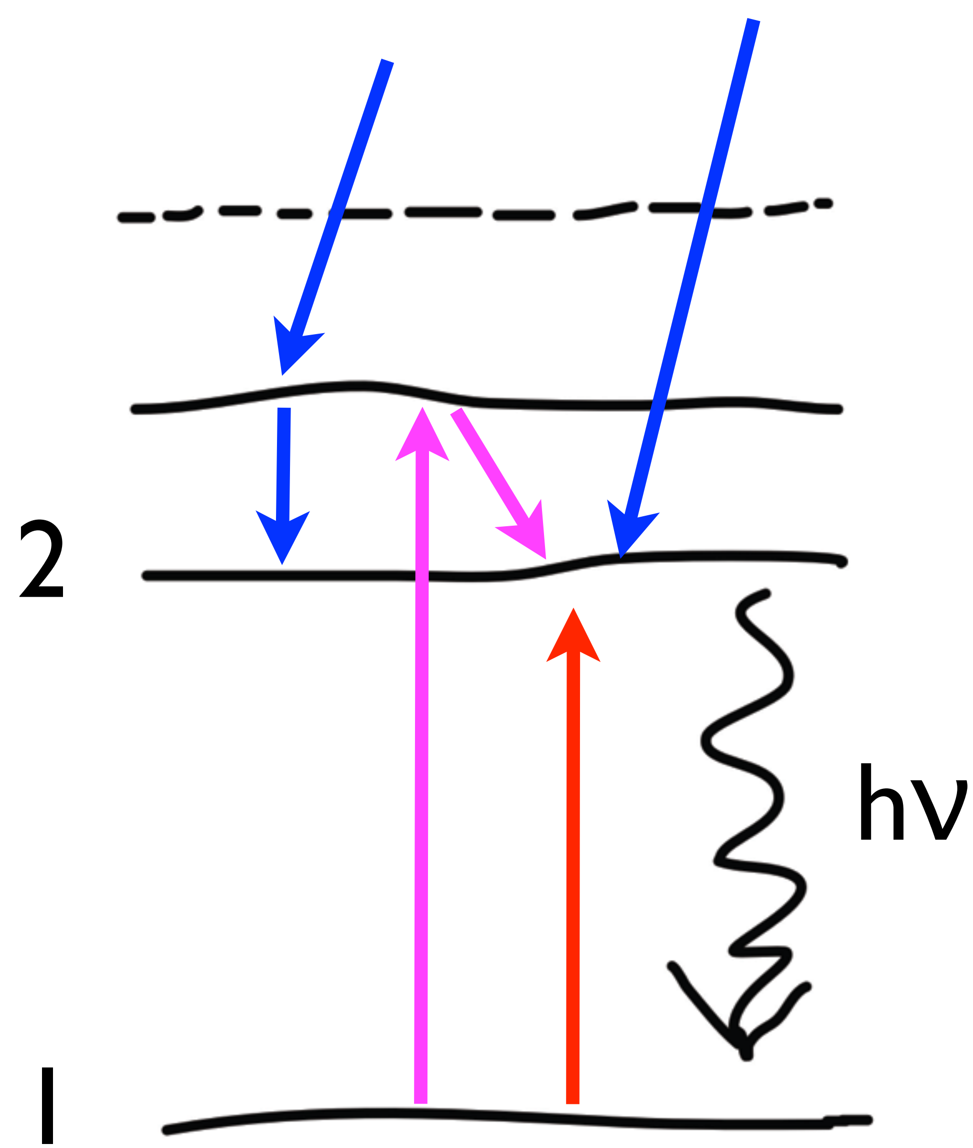
dashed: ionization balance according to Mazzotta *et al.* 1998
solid: according to Bryans *et al.* 2006,9

kT = 1 keV, Solar abundances,
different ionization balances, line emissivities

Foster *et al.*, ApJ, 2012

emission line spectrum

gas density very low, radiation field very dilute, plasma optically thin:
all ions are in the ground state *because radiative decay much faster than collisional processes*

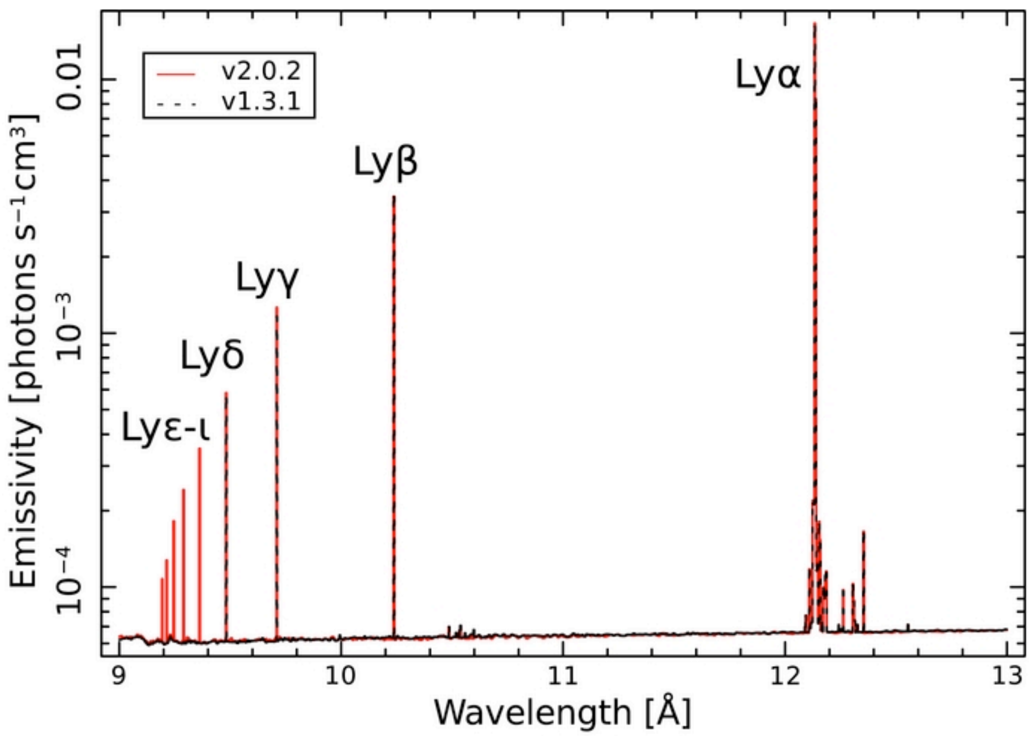


whatever process populates n = 2, it always results in a photon 2 → 1

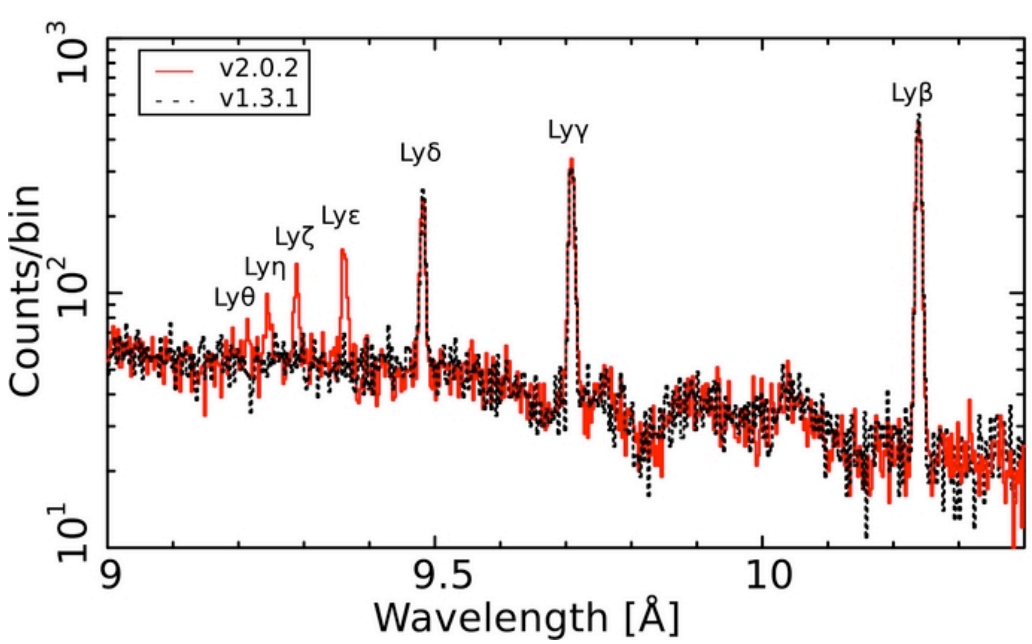
this is peculiar to X-ray transitions (the spontaneous radiative decays are fast)

emission line spectrum

therefore, the main difficulty is calculating the rates for all the processes that populate the upper level !



example for Ne X; $T = 10^7$ K;
in some cases, recombination onto higher levels produces significantly higher flux in low-order series members

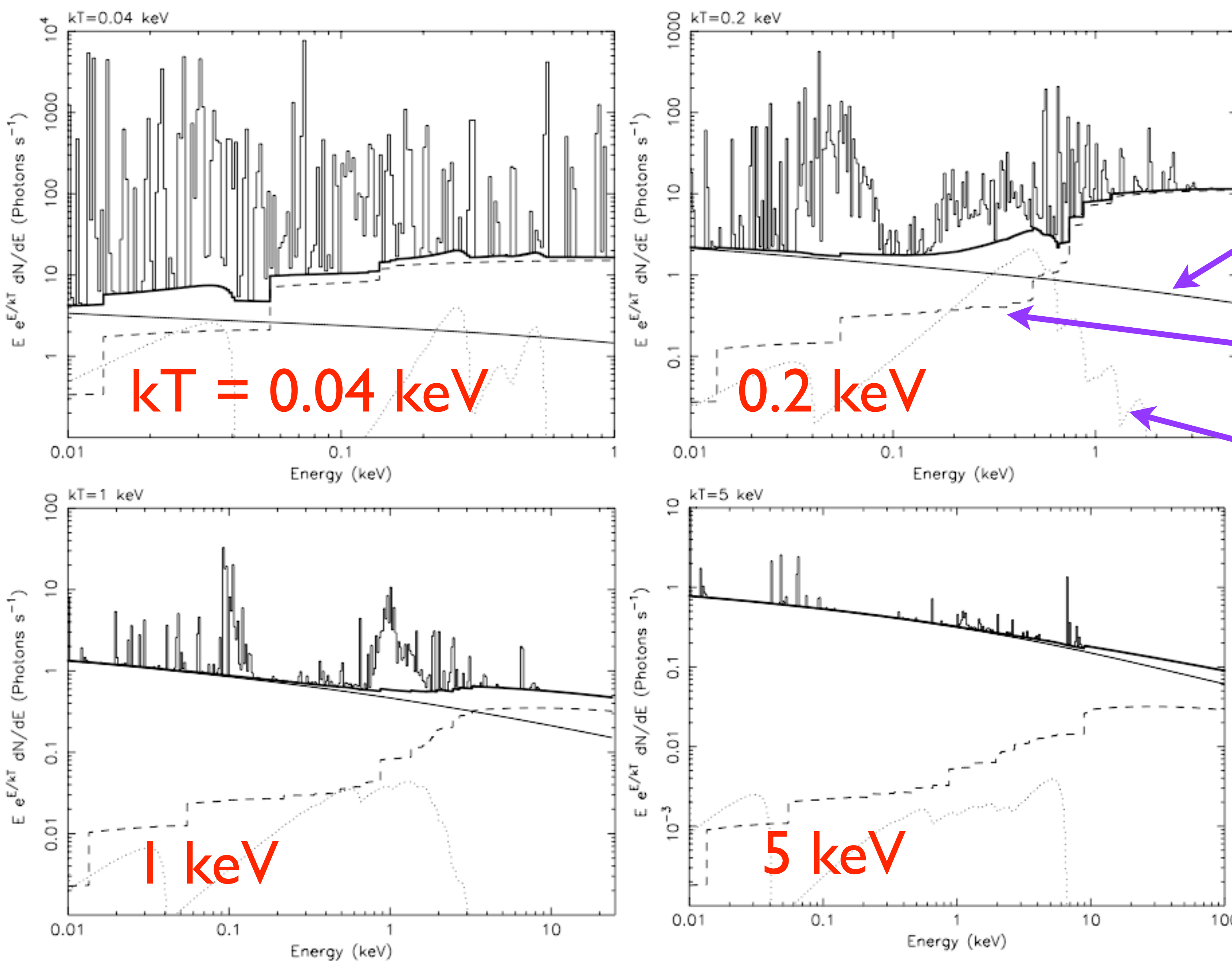


there is more to collisional plasmas than simple collisional excitation!

Foster *et al.* 2012

continuum emission spectrum

electron-proton (-ion) bremsstrahlung ('free-free')
recombination emission ('free-bound')
2s-1s two-photon emission (!!)



brems

recombination

two-photon
(note how important this can be at low kT!)

Kaastra *et al.* 2008

specific spectroscopic diagnostics

1. 'charge state spectroscopy': temperature; degree of equilibration

H/He-like

X-ray plasma

Fe L series

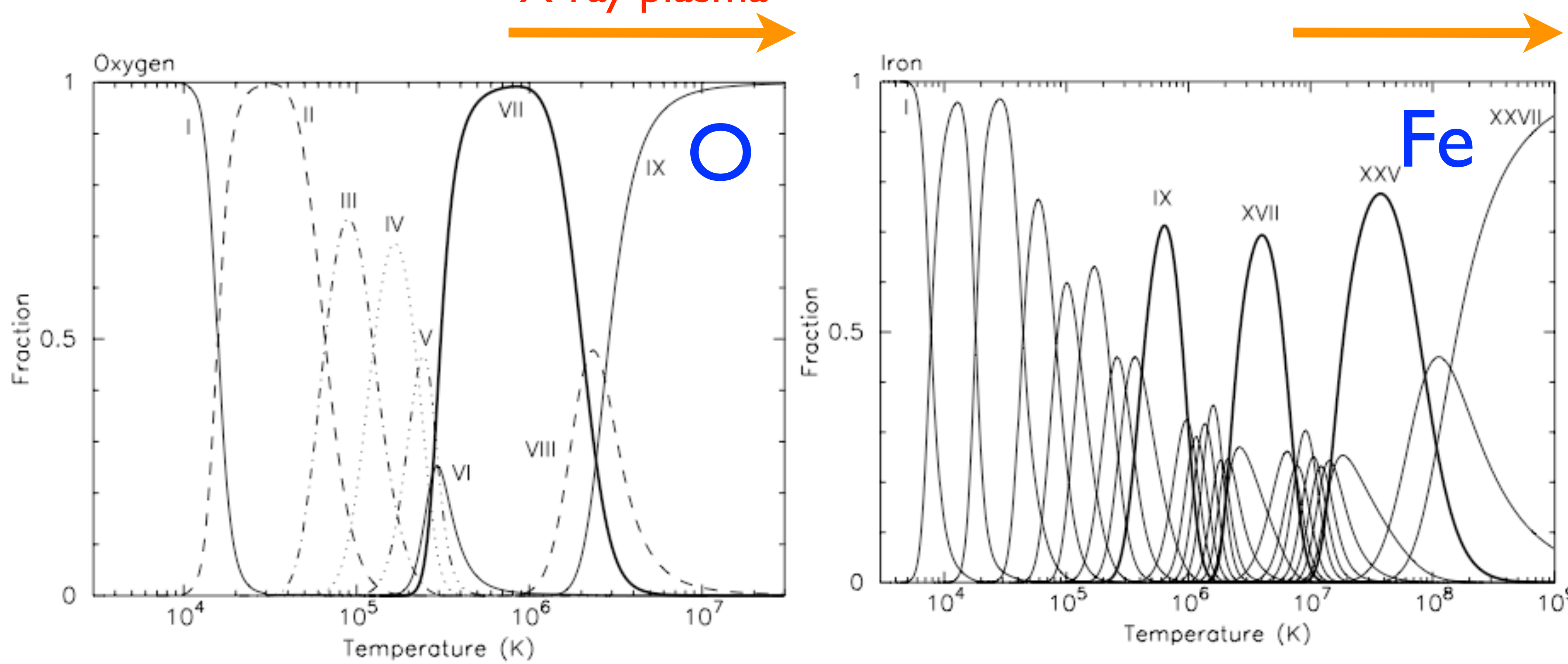


Fig. 7 Ion concentration of oxygen ions (*left panel*) and iron ions (*right panel*) as a function of temperature in a plasma in Collisional Ionisation Equilibrium (CIE). Ions with completely filled shells are indicated with *thick lines*: the He-like ions O VII and Fe XXV, the Ne-like Fe XVII and the Ar-like Fe IX; note that these ions are more prominent than their neighbours

another representation of the Fe L series

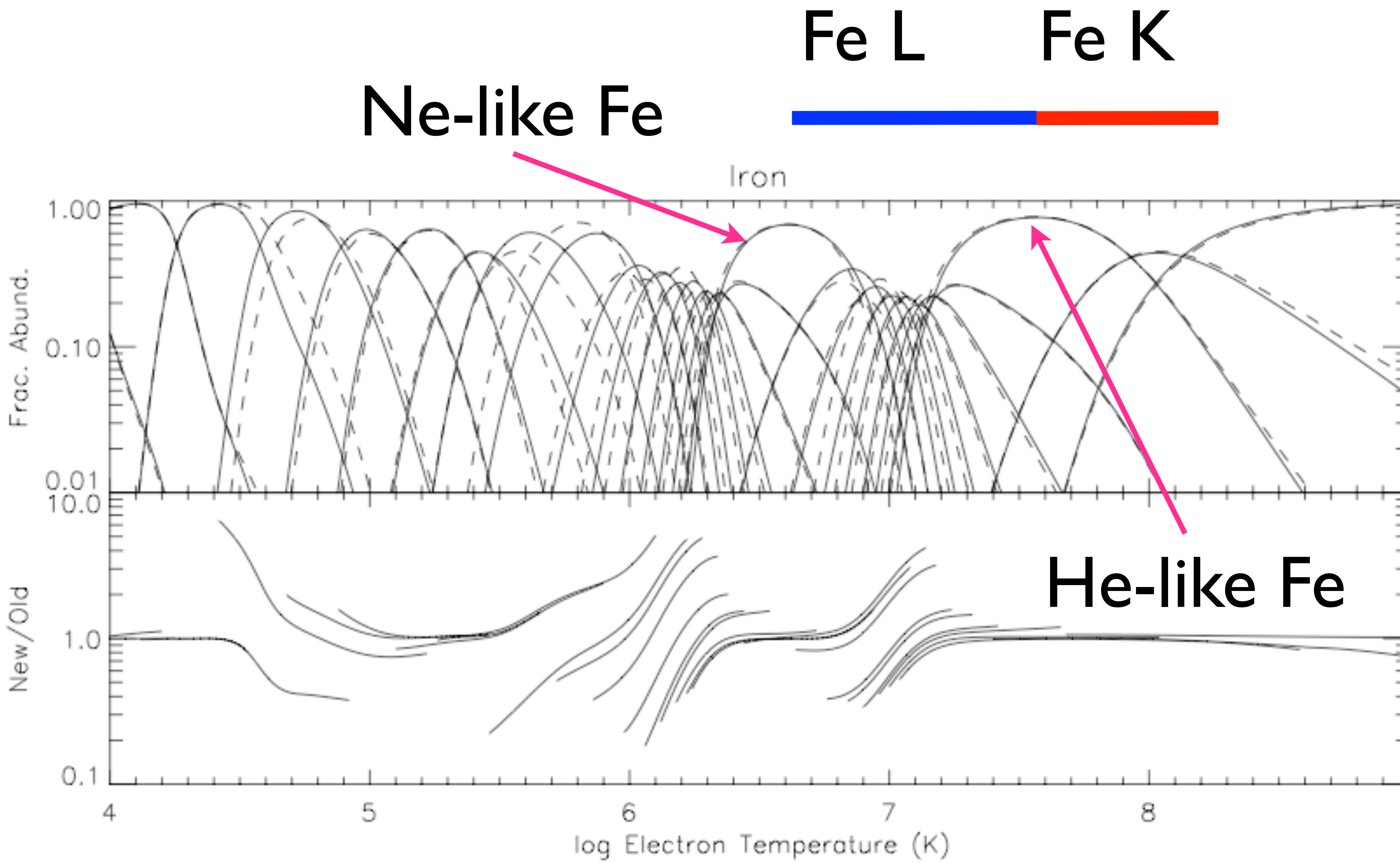
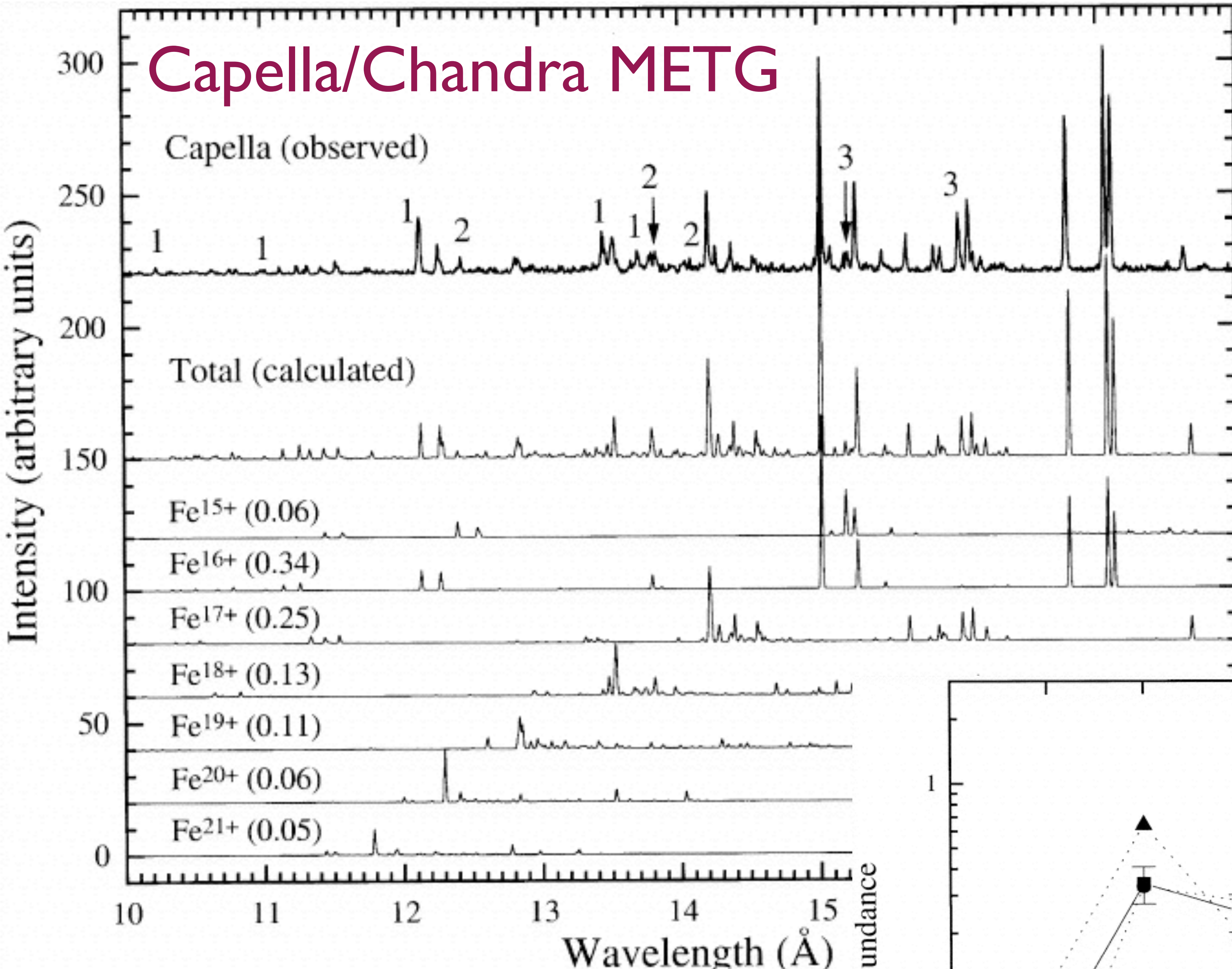


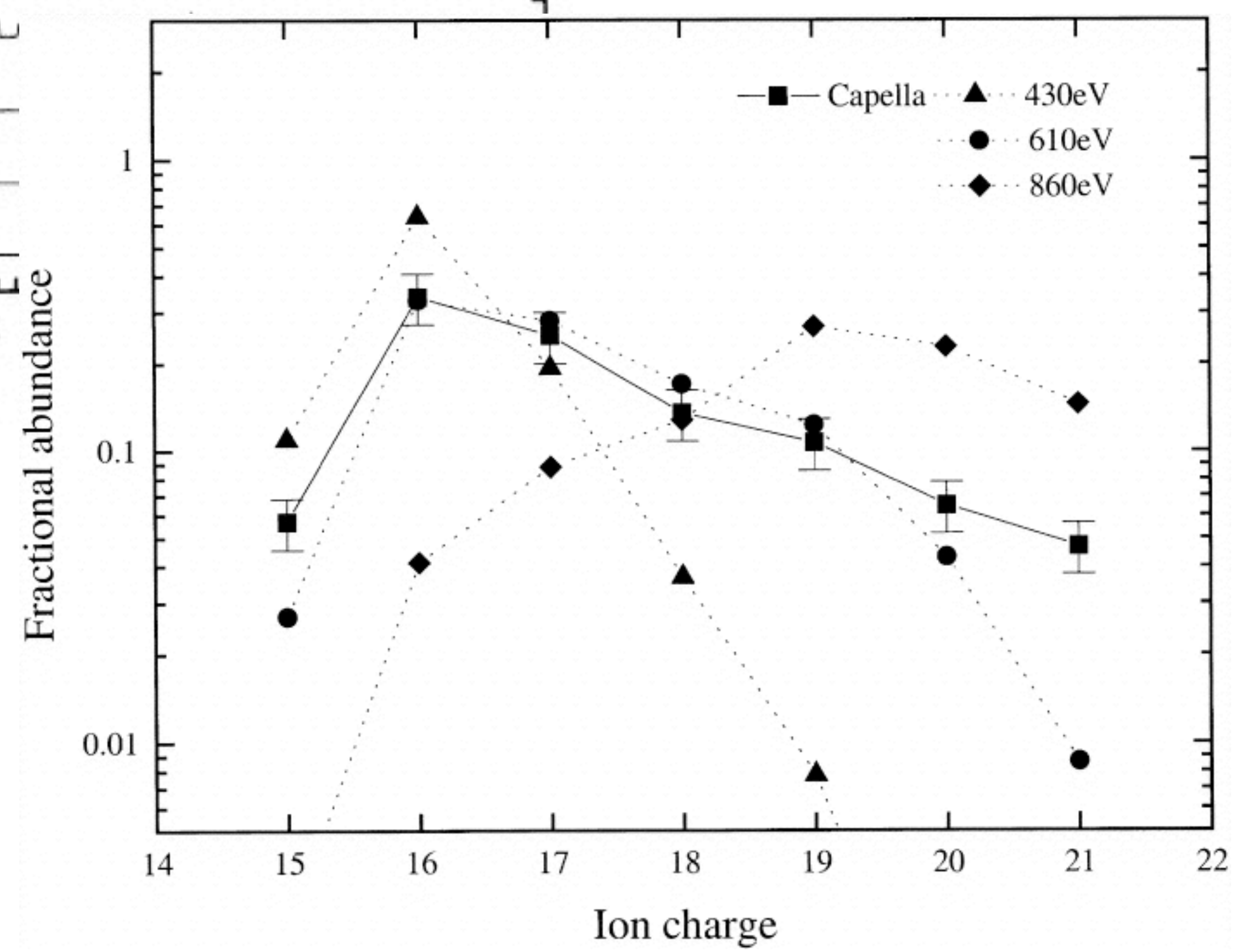
Figure 1. Ionization fractional abundance vs. T_e for all ionization stages of Fe. The upper graph shows our results (solid curves) and the abundances calculated by Mazzotta et al. (1998; dashed curves). The lower graph shows the ratio of the calculated abundances. Comparison is made only for fractional abundances greater than 10^{-2}. We label our results as "New" and those of Mazzotta et al. (1998) as "Old."

Bryans *et al.* 2009

Capella/Chandra METG

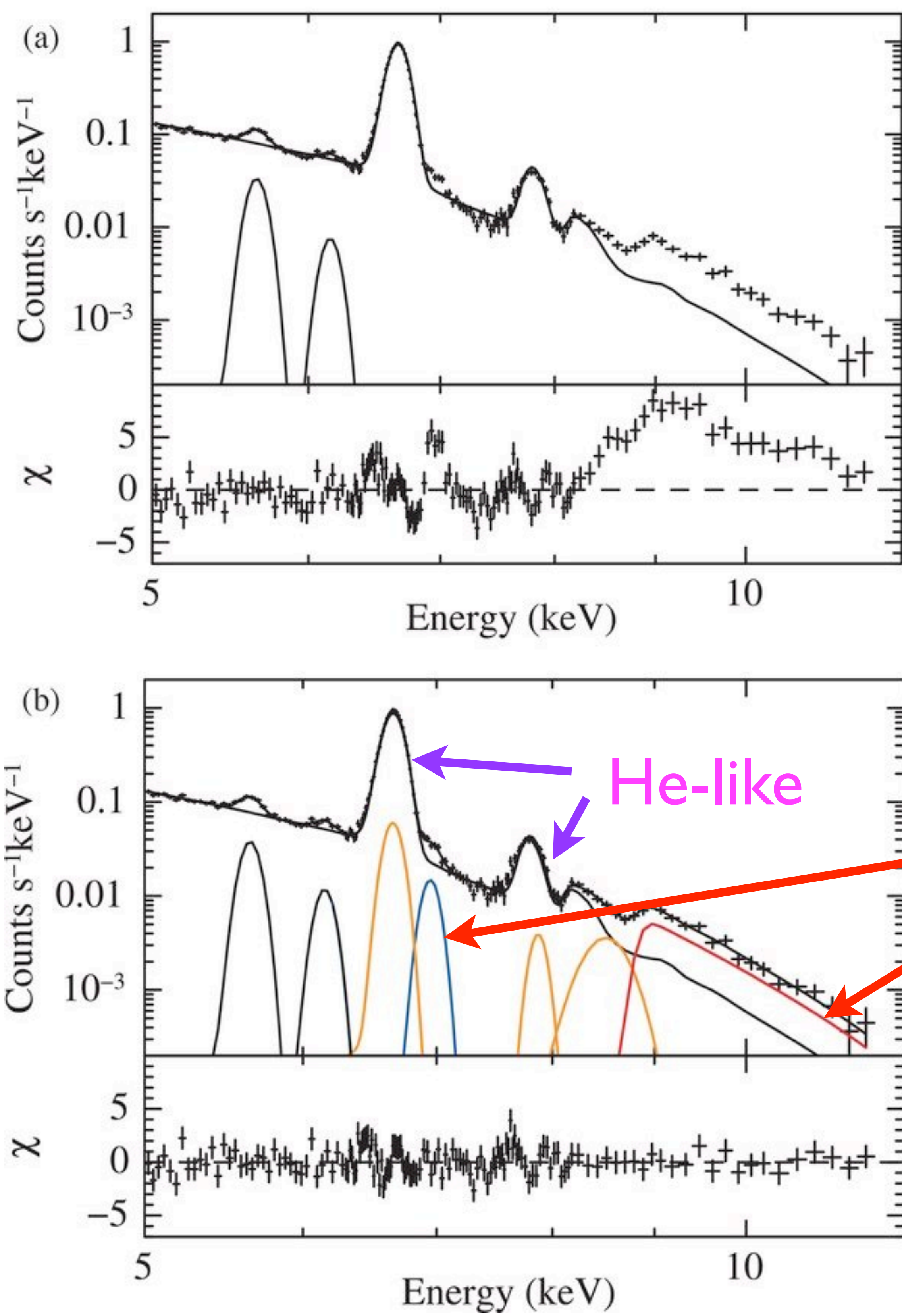


Behar, Cottam, Kahn 2009



‘charge state spectroscopy’: degree of equilibration

Figure 3 from M. Ozawa et al. 2009 ApJ 706 L71



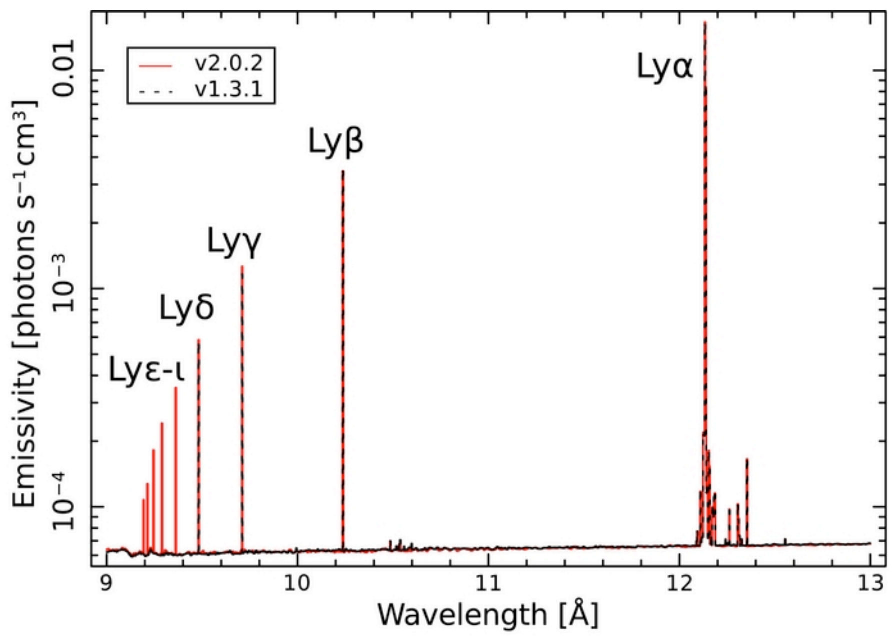
SNR W49B/Suzaku
Ozawa *et al.* 2009

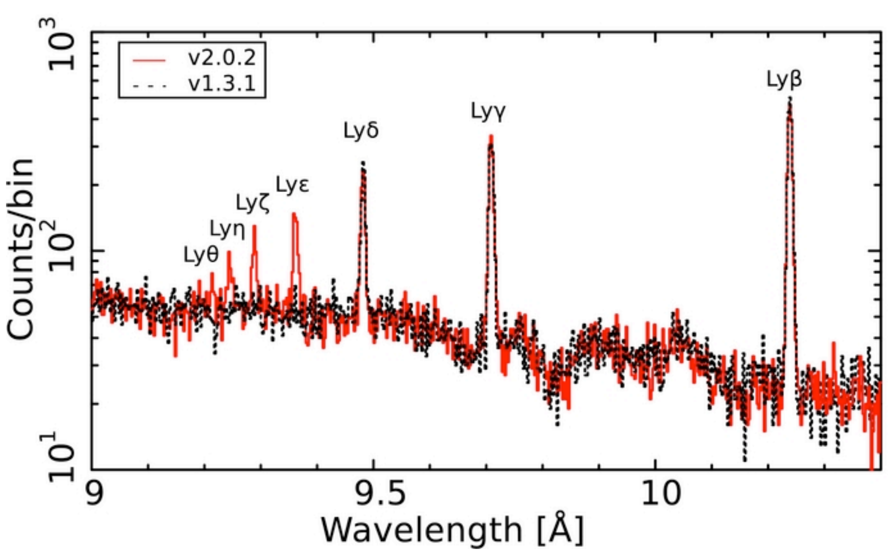
direct measurement of H/He-like Fe abundance: ratio does *not* match predicted value for measured T_e !

huge overabundance of H-like!

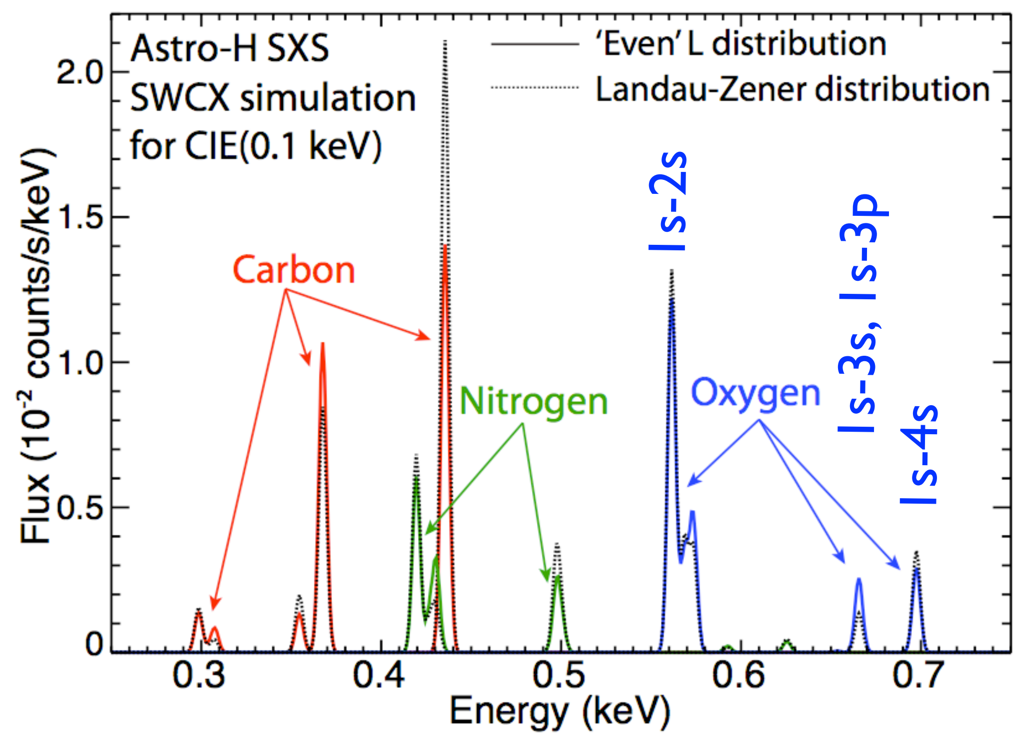
2. Series 'Decrement(*)': excitation mechanism

CX





not CX



ratio n = m-1/2-1 sensitive to excitation mechanism (CX or recombination-dominated)

(the other very strong diagnostics are the appearances of the RRC and the He-like triplets)

(*) from 'to decrease'

3. He-like ions:
density, temperature, radiation fields, optical depth

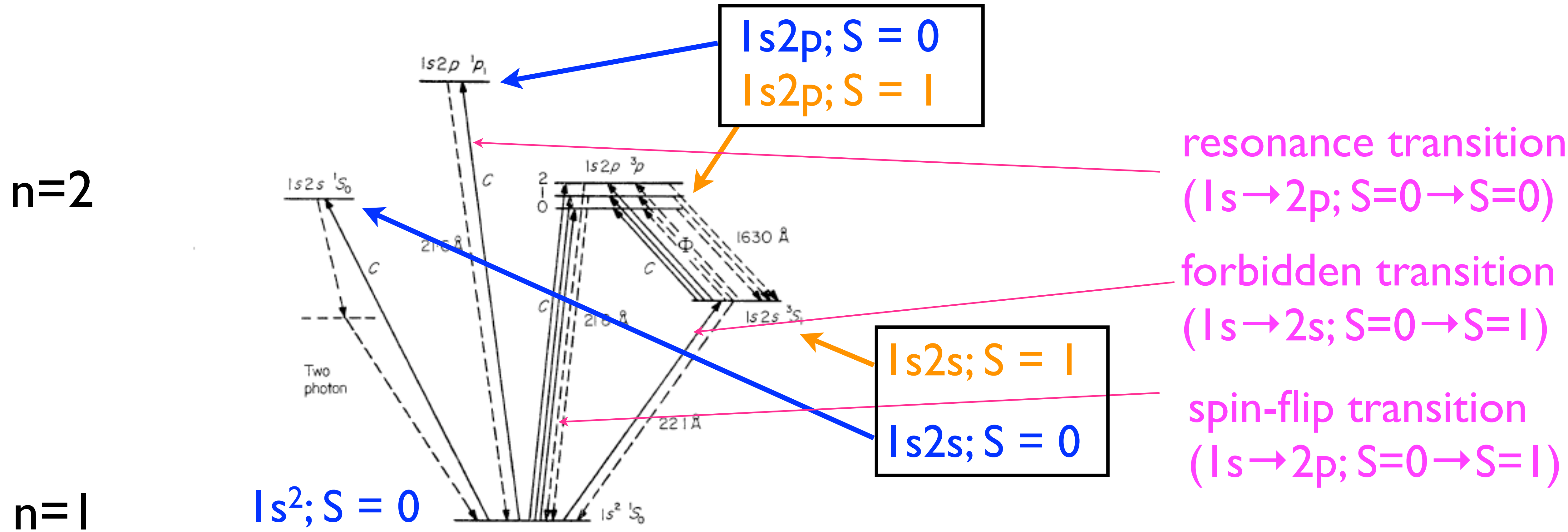


FIG. 1. *The He-like ion, showing those terms and processes involved in the present analysis. The wavelengths indicated apply to the case of oxygen* VII.

two electrons: wave function = spatial($\mathbf{r}_1$,$\mathbf{r}_2$) x spin(s_1,s_2)

has to be antisymmetric: symmetric x antisymmetric
antisymmetric x symmetric

spin wave function: |↑↑> , |↑↓> + |↓↑>, |↓↓>, and |↑↓> - |↓↑>

symmetric; S = 1 — *triplet*

antisymmetric; S = 0 — *singlet*

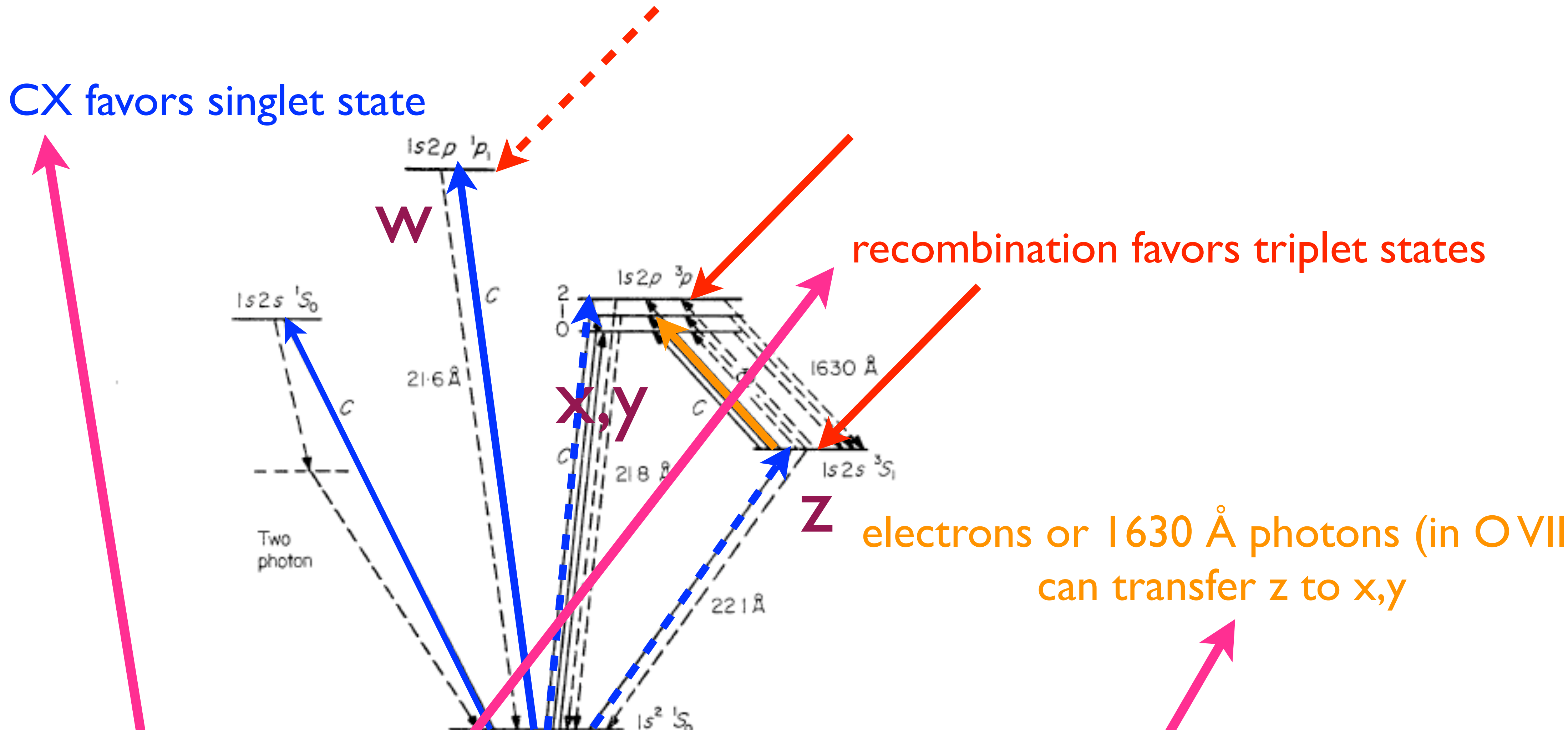


FIG. 1. *The He-like ion, showing those terms and processes involved in the present analysis. The wavelengths indicated apply to the case of oxygen* VII.

Gabriel and Jordan 1969

collisional excitation and recombination
have different *T*-dependence

ratio x,y to z density (or UV field) sensitive

He-like Oxygen ‘critical density’

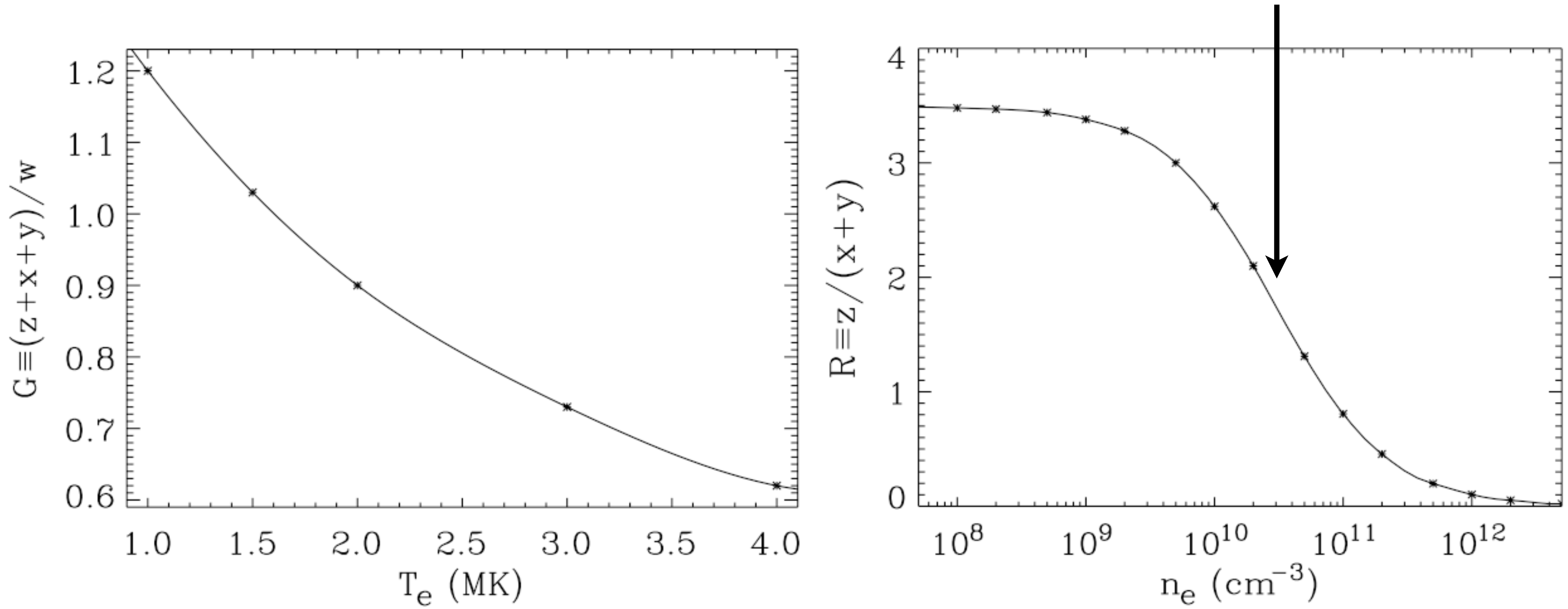


Fig. 8 Electronic temperature (T_e) and density (n_e) plasma diagnostics for the He-like O VII ion. *Left panel:* $\mathcal{G} \equiv (z + x + y)/w$ versus T_e for $n_e = 10^{10}$ cm^{-3}. *Right panel:* $\mathcal{R} \equiv z/(x + y)$ versus n_e for $T_e = 10^6$ K. Calculations are taken from Porquet et al. (2001a)

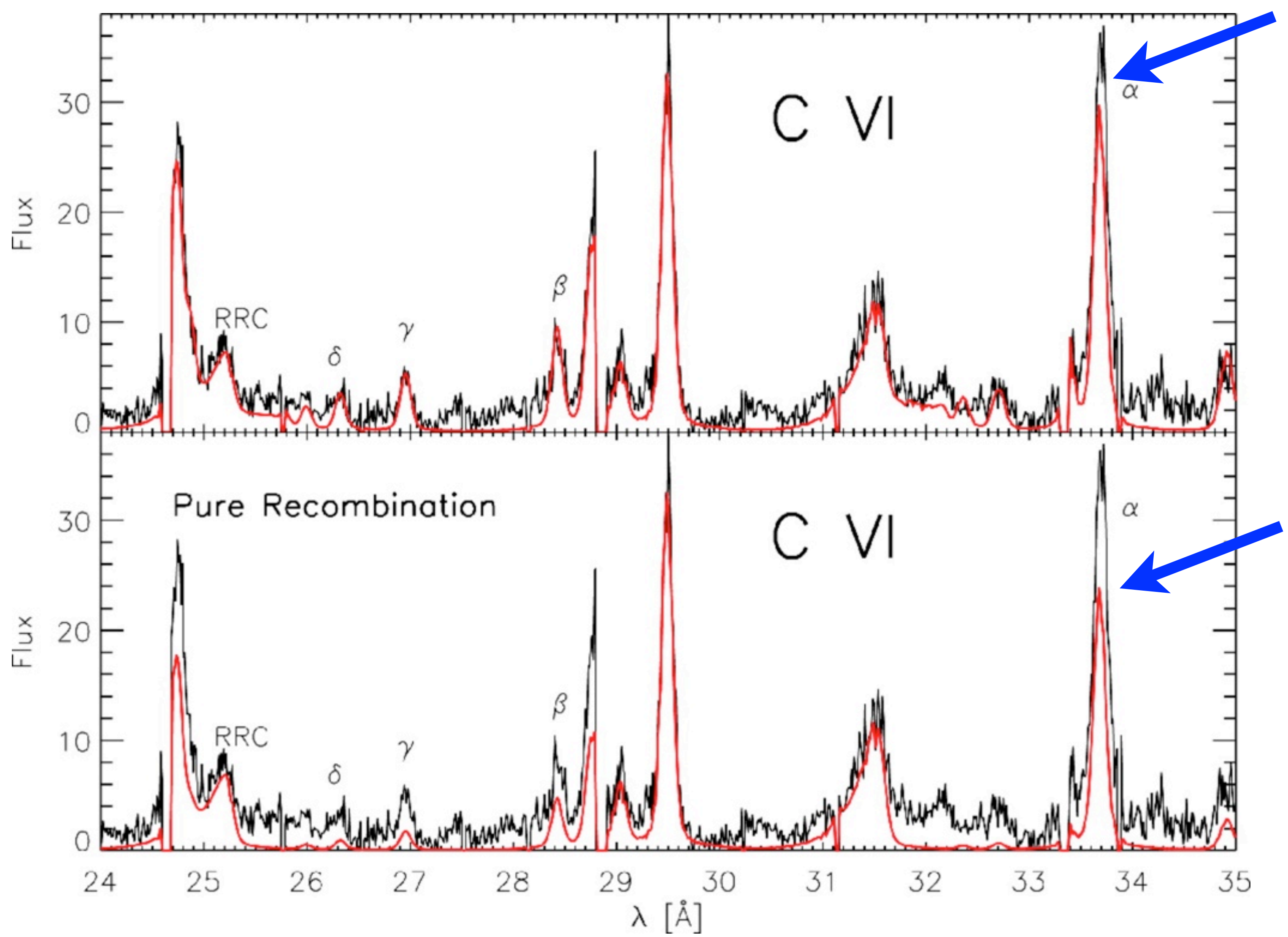
from Porquet *et al.* Space Sci Rev, **157** (2010)

and similarly for He-like C, N, Ne, Mg, Si, S, Ar, Ca, Fe; ever increasing critical density

not sure there is always a unique solution (T_e,n_e) ?
also: source often not isothermal (isochoric)

He-like triplets also sensitive to X-ray radiation field and optical depth:

w enhanced by photoexcitation:
continuum photon of energy coincident with *w* can be scattered



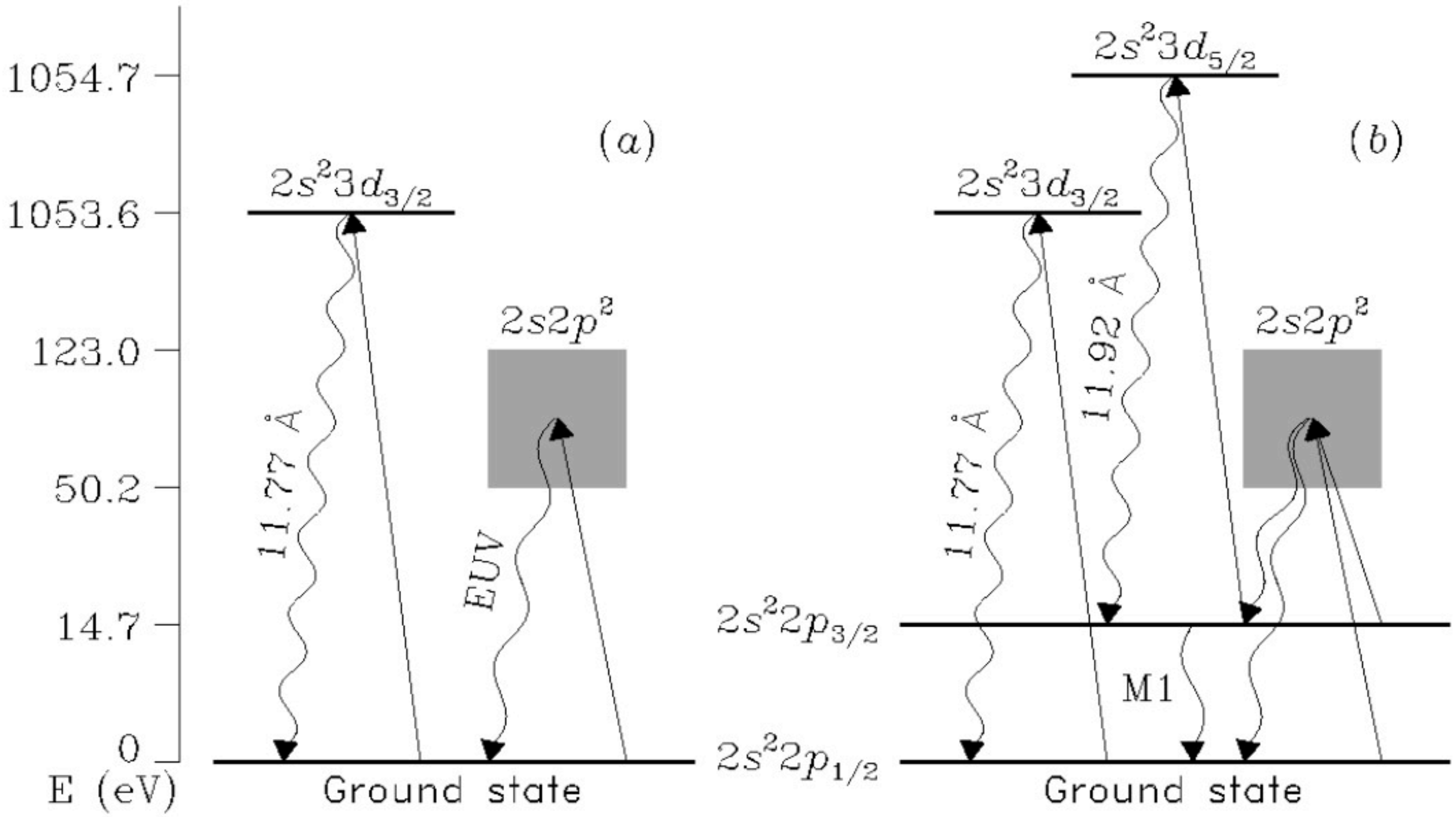
resonance line photons are being scattered into our line of sight

though this is H-like;
and it is not a CIE source-
but I know of no CIE example !

NGC1068;
Kinkhabwala *et al*. 2002

4. Density diagnostics in Fe L series

example: Fe XXII 11.77/11.92 Å ratio



ground: $1s^22s^22p_{1/2}$

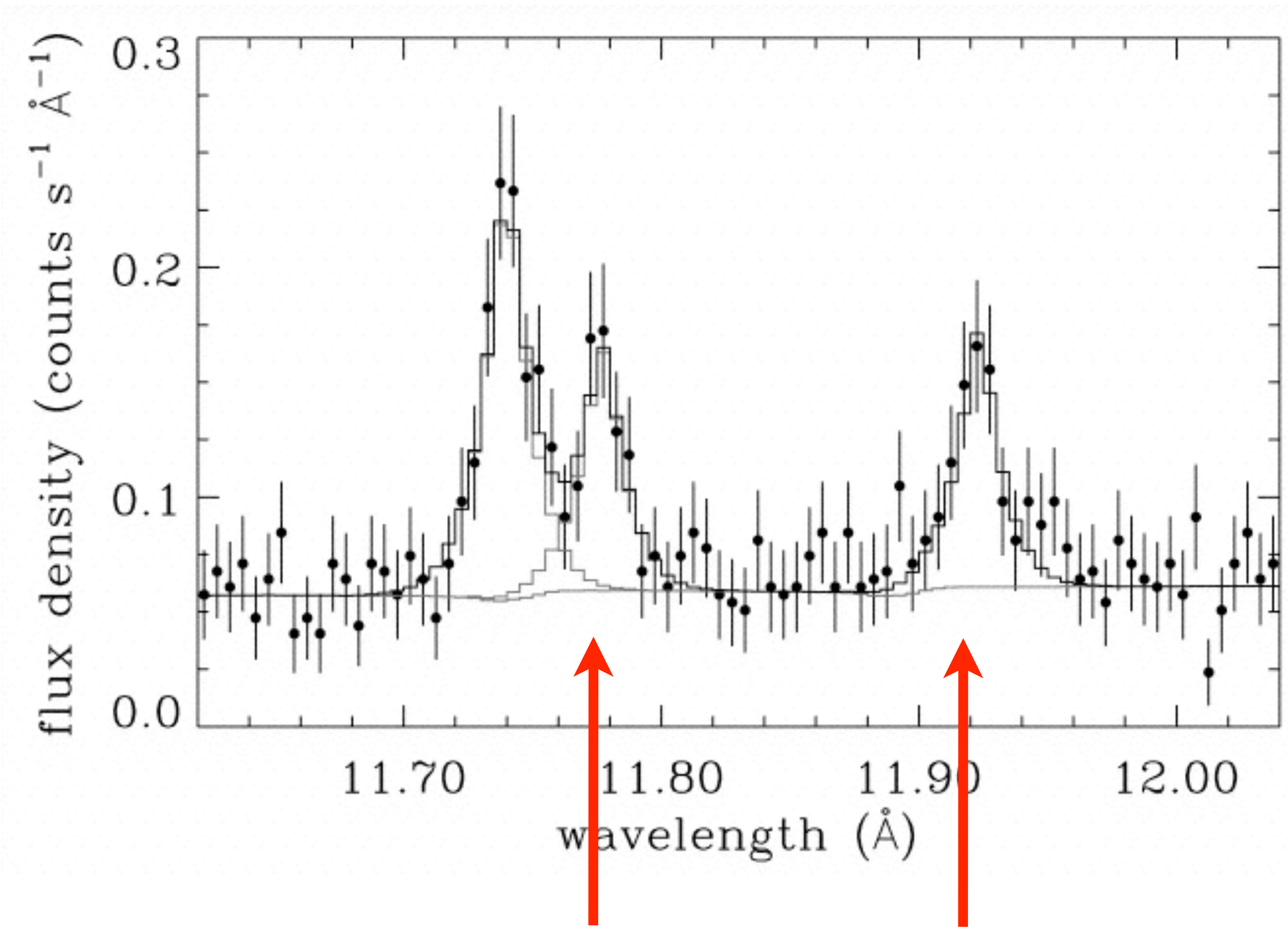
low density

high density: $2s^22p_{3/2}$ populated; 11.92 Å appears

Mauche, Liedahl, Fournier, *ApJ*, 2003

4. Density diagnostics in Fe L series

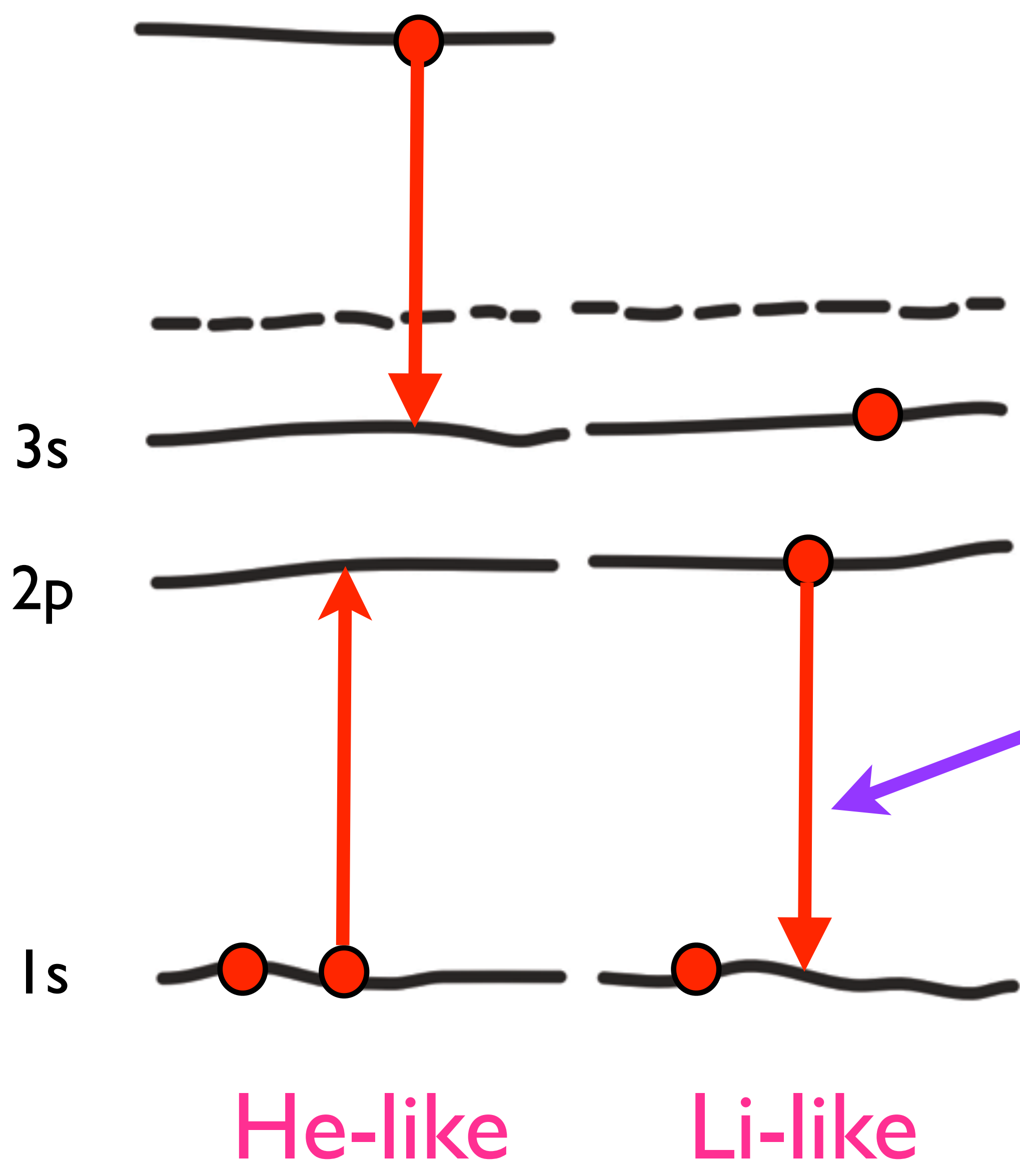
example: Fe XXII 11.77/11.92 Å ratio



EX Hya, *Chandra* HETGS

5. Dielectronic Satellites

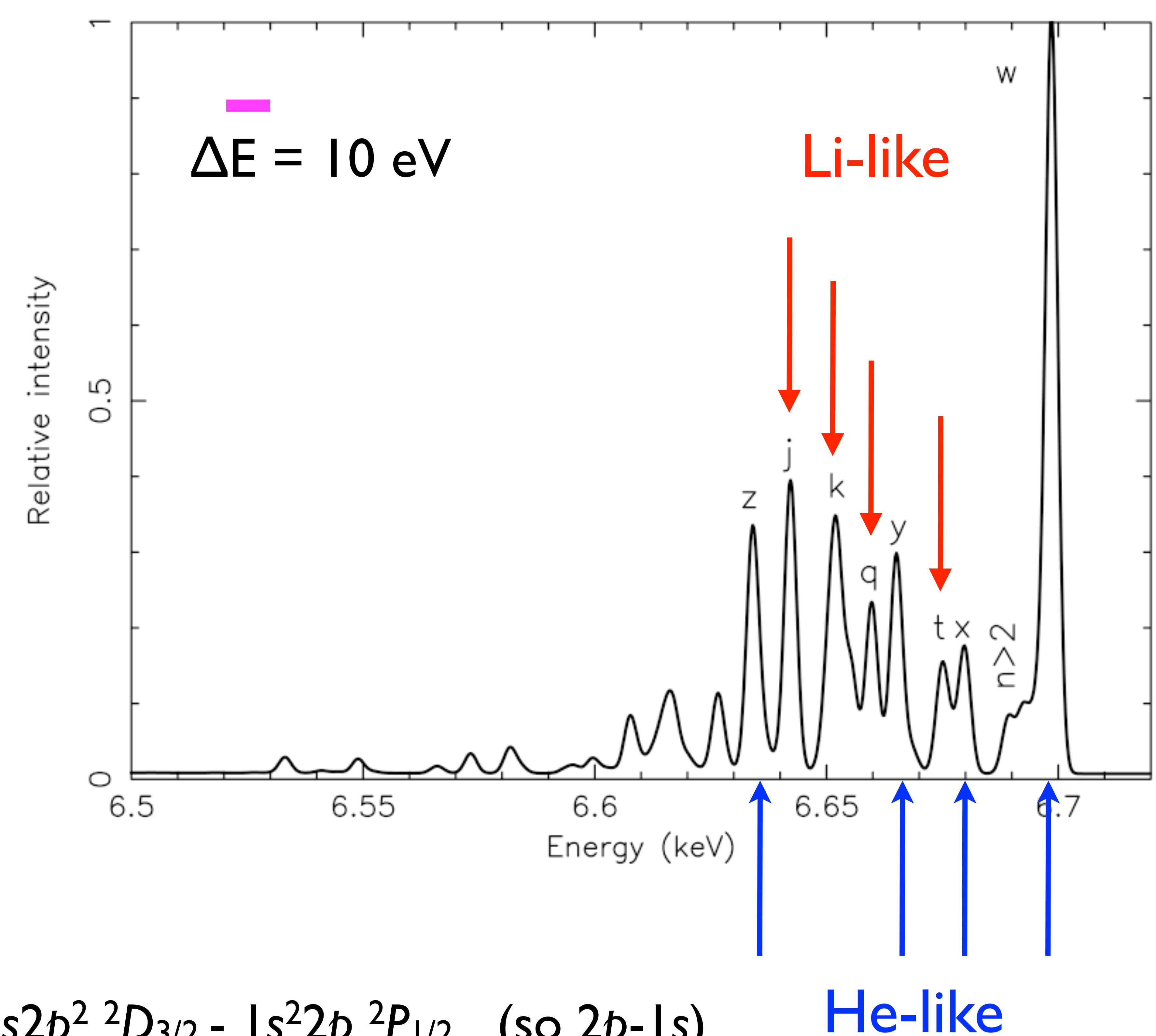
source for *both* the satellite and the parent line is the He-like ion: ratio does not involve ionization balance! but it ***is*** sensitive to temperature (through CX and DR rates)!



n=2-1, energy slightly lower than corresponding line in He-like: 'satellite' to the He-like 'parent' line

dielectronic recombination

Li-like/He-like Fe; kT_e = 2 keV



ex.: k: $1s2p^2\ ^2D_{3/2}$ - $1s^22p\ ^2P_{1/2}$ (so $2p$-$1s$)

q: $1s2p(^3P)2s\ ^2P_{3/2}$ - $1s^22s\ ^2S_{1/2}$ (so $2p$-$1s$)

Kaastra *et al.* 2008