

# First Astro-H Science Summer School

Minakami Onsen, August 19-21, 2010

## 1. Radiation Processes

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# Atomic Structure

## The Bohr Atom

clue to significance of principal quantum number ('shells', in multi-electron systems)  
useful scaling with nuclear charge



Quantize angular momentum  $L$  of electron  
in circular orbit around nucleus of charge  $+Ze$ :

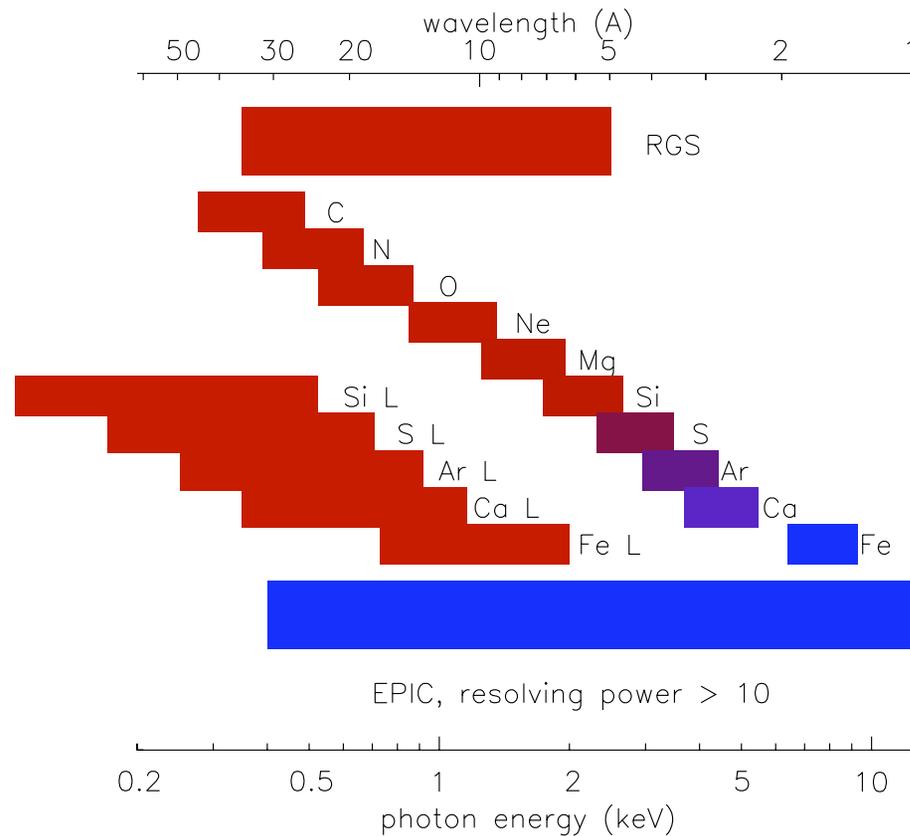
$$L = m_e v r = n \hbar$$

You find for the allowed energies:

$$E_n = -\frac{Z^2 \mathcal{R}}{n^2}; \quad n = 1, 2, 3, \dots$$

$\mathcal{R}$ : the Rydberg Constant,  $\mathcal{R} = 13.606$  eV

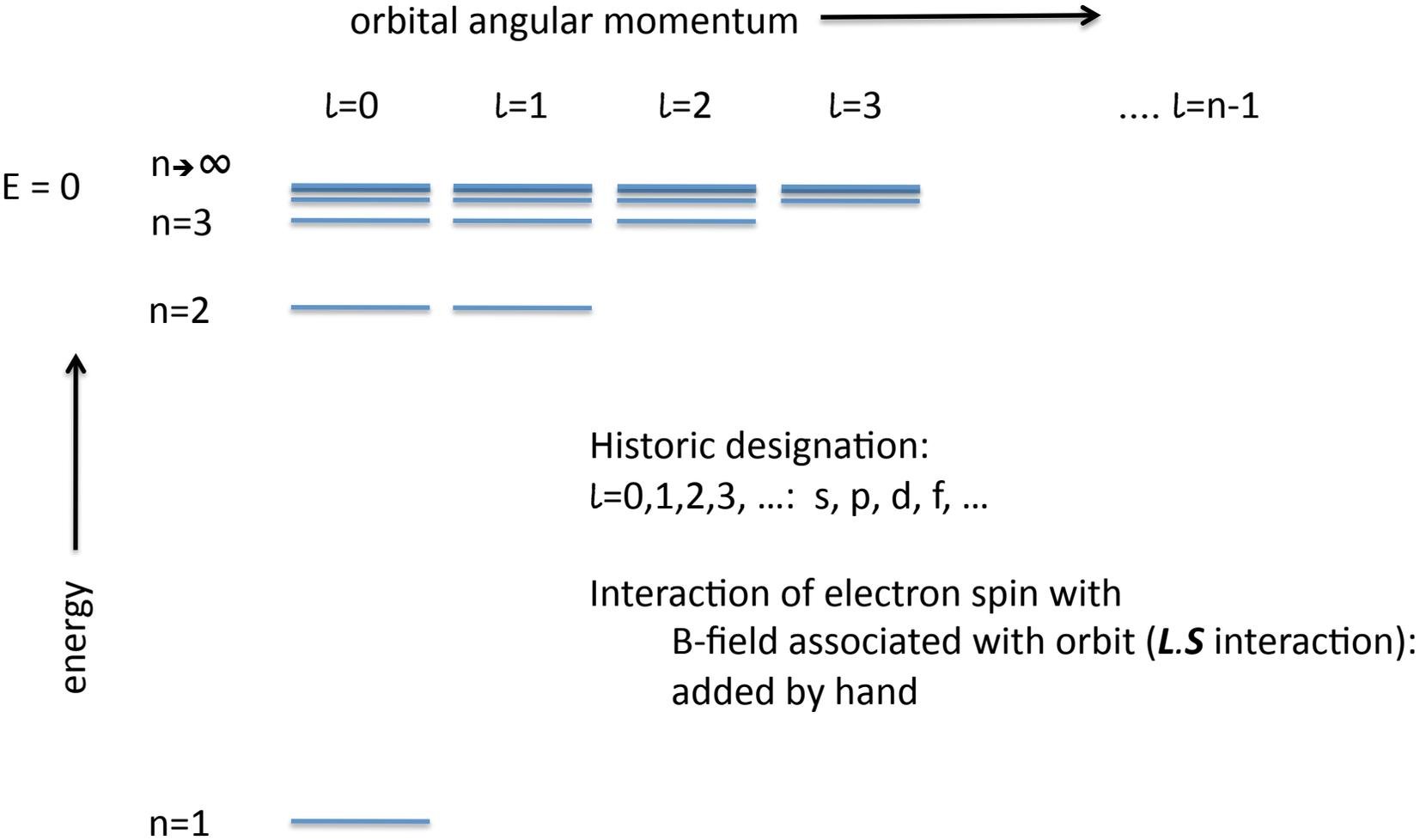
## X-ray spectra of the abundant elements



X-ray spectra, between neutral fluorescent  $n=2-1$ , and H-like  $n=1-\infty$ ,  
estimated from  $E = -Z^2R/n^2$

Never leave home without the Bohr model!

**Non-relativistic Approximation:  
Schroedinger's Equation for single electron in Coulomb potential**



## Relativistic Systems:

Dirac Equation; electron spin appears automatically;  $L.S$  coupling automatically included

One electron in Coulomb field:

$$\frac{E_n}{m_e c^2} = \left\{ 1 + \left( \frac{\alpha Z}{n - k + \sqrt{k^2 - \alpha^2 Z^2}} \right)^2 \right\}^{-1/2} - 1$$

$$E_n \approx \frac{-Z^2 \mathcal{R}}{n^2} \left\{ 1 + \frac{(\alpha Z)^2}{n} \left( \frac{1}{k} - \frac{3}{4n} \right) \right\}$$

$n = 0, 1, 2, 3, \dots$ ;  $k = 1, 2, \dots, n$ ;  $\alpha \approx 1/137$ , the fine structure constant

Relativistic effects important if  $E_n/m_e c^2 > 10^{-3}$ : that means:  $Z > 6$  (Carbon) !!!

**Always** important for Astro-H spectroscopy!!



## Spectroscopic Notation

$L, l, S, s$ : vectors!

Add all electron orbital angular momenta,  $L = \sum l_i$  ; label S, P, D, F, ...

Add all electron spin angular momenta,  $S = \sum s_i$

The  $2S + 1$  states with the same total spin  $S$  are distinguished by their *total* angular momentum  $J$ :

Level notation:  $^{2S+1}L_J$  ;

sets of levels ("terms") with  $2S+1 = 1, 2, 3, \dots$  are called singlets, doublets, triplets, ...

Example: two electrons in  $n=3, l=1$ :  $3p^2$ . That means:  $l = 1, s=1/2$  for both e's

Possible values of  $L$ :  $L = l_1 + l_2$ , so  $L = 0, 1, \text{ or } 2$  (S, P, and D)

Possible values of  $S$ :  $S = s_1 + s_2$ , so  $S = 0$  or  $1$

Possible terms:  $^1S, ^3P, ^1D$

(nb: total wavefunction has to be antisymmetric. So, for example,  $^3S$  not allowed because S states ( $L=0$ ) are spatially symmetric; need antisymmetry in spins)

The  $^3P$  has three J-states:  $J = L + S = 0, 1, 2$ , so  $^3P_{0,1,2}$

Reminder: correct addition of two electron spins (important for He-like ions!!):

Four possible combinations of two electron spins (up or down,  $s = +1/2$  or  $s = -1/2$ ):

$$|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle.$$

Of these,  $|\uparrow\uparrow\rangle$  and  $|\downarrow\downarrow\rangle$  are eigenfunctions of the total spin operator (so are stationary spin states);  $|\uparrow\downarrow\rangle$  and  $|\downarrow\uparrow\rangle$  are not. But the two linear combinations  $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$  and  $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$  are eigenfunctions.

So four possible spin states:

$$\begin{array}{l} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{array} \quad \text{the triplet states: all three } S = 1: \text{ symmetric in spins.}$$

and

$$|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \quad \text{the singlet state: } S = 0: \text{ antisymmetric in spins.}$$

# Line Radiation: Classical, Quantum

Best short introduction: S. M. Kahn: *'Soft X-ray Spectroscopy of Astrophysical Plasmas'*,  
(see bibliography at the end)

## Classical

Solution to Maxwell's equations for given charges  $\rho(\mathbf{r},t)$  and currents  $\mathbf{j}(\mathbf{r},t)$ :

$$\varphi(\mathbf{r}, t) = \int d^3\mathbf{r}' dt' \frac{\rho(\mathbf{r}', t')}{|\mathbf{r} - \mathbf{r}'|} \delta [t' - t_r(\mathbf{r}, t, \mathbf{r}')] ,$$
$$\mathbf{A}(\mathbf{r}, t) = \int d^3\mathbf{r}' dt' \frac{\mathbf{j}(\mathbf{r}', t')}{|\mathbf{r} - \mathbf{r}'|} \delta [t' - t_r(\mathbf{r}, t, \mathbf{r}')]$$

with retarded time

$$t_r \equiv t - \frac{|\mathbf{r} - \mathbf{r}'|}{c}$$

Fourier transform  $\mathbf{j}(\mathbf{r}, t)$  and  $\mathbf{A}(\mathbf{r}, t)$ , and inspect solution for  $\tilde{\mathbf{A}}(\mathbf{r}, \omega)$  far from source ( $r \gg r'$ ):

$$\tilde{\mathbf{A}}(\mathbf{r}, \omega) \approx \frac{e^{ikr}}{rc} \int d^3\mathbf{r}' \tilde{\mathbf{j}}(\mathbf{r}', \omega) e^{-ik(\hat{\mathbf{n}} \cdot \mathbf{r}')}$$

( $\hat{\mathbf{n}}$  unit vector, points in direction of  $\mathbf{r}$ ).

Expand  $\exp(-ik(\hat{\mathbf{n}} \cdot \mathbf{r}'))$  ("Multipole expansion"), and assume  $k(\hat{\mathbf{n}} \cdot \mathbf{r}') \ll 1$ ; condition is equivalent to  $v/c \ll 1$  (source nonrelativistic).

Keep first term ("electric dipole term", "E1"); gives  $\tilde{\mathbf{A}}(\mathbf{r}, \omega)$  in terms of (Fourier transform of) dipole moment of charge distribution,  $\mathbf{d}(\omega)$ . Calculate  $\mathbf{E}(\mathbf{r}, \omega)$  and  $\mathbf{B}(\mathbf{r}, \omega)$  from  $\tilde{\mathbf{A}}(\mathbf{r}, \omega)$ , and transform back to  $t$ . From the Poynting vector,  $\mathbf{S}$ , calculate the radiated power,  $dW/dt$ :

$$\frac{dW}{dt} = \int \mathbf{S} r^2 d\Omega = \frac{2}{3} \frac{|\ddot{\mathbf{d}}|^2}{c^3}$$

For a single oscillating charge, subject to acceleration  $a$ , you get the Larmor formula:

$$\frac{dW}{dt} = \frac{2}{3} \frac{q^2 a^2}{c^3}$$

Note: higher order terms in multipole expansion are smaller than dipole term by factors  $(v/c)^2$ .

Simple classical model for atomic line radiation now follows from considering a simple bound, damped harmonically oscillating charge; see Kahn for details.

Example: the classical decay rate,  $(dW/dt)/W_0$ , of the classical harmonic oscillator:

$$A_{cl} \equiv \frac{(dW/dt)}{W_0} = \frac{2}{3} \frac{q^2 \omega_0^2}{mc^3}$$

This scales like (frequency)<sup>2</sup>; in the X-ray band, frequencies are of order  $\nu \sim 10^{16-18}$  Hz, A is of the order  $10^{10-14} \text{ sec}^{-1}$  !

## Quantum mechanics (quantized atomic structure; classical radiation field)

Atomic structure given by solutions to Schrodinger equation:

$$\mathcal{H} |\psi\rangle = E |\psi\rangle$$

with  $\mathcal{H}$  the Hamiltonian for the system of bound electrons.

Interaction with radiation represented by adding a small perturbation to  $\mathcal{H}$ :

$$\mathcal{H} = \mathcal{H}^0 + \Delta\mathcal{H}$$

and applying time-dependent first order perturbation theory.

The probability per unit time that atomic electron system will make transition from stationary state  $|n\rangle$  to state  $|n'\rangle$  given by

$$R = \frac{2\pi}{\hbar} |\langle n' | \Delta\mathcal{H} | n \rangle|^2 \delta(E_{n'} - E_n \pm \hbar\omega)$$

The  $\delta$ -function ensures that transitions only occur for radiation of frequency  $\omega$ :  
 $\hbar\omega = E_{n'} - E_n$  (one photon).

The 'radiation Hamiltonian',  $\Delta\mathcal{H}$ :

Classical Hamiltonian of particle in  $\mathbf{A}$ -field:

$$\mathcal{H} = \frac{1}{2m} \left( \mathbf{p} - \frac{q}{c} \mathbf{A} \right)^2 + q\phi$$

Transition to quantum mechanics:  $\mathbf{p} \rightarrow (\hbar/i)\nabla$  ;  $\phi = 0$  in a radiation field,  
and you can choose  $\text{div } \mathbf{A} = 0$ .

Discard term in  $\mathbf{A}\cdot\mathbf{A}$ , add atomic Coulomb potential  $V(\mathbf{r})$ , get

$$\mathcal{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + \frac{iq\hbar}{mc} (\mathbf{A} \cdot \nabla)$$

so

$$\Delta\mathcal{H} = \frac{iq\hbar}{mc} (\mathbf{A} \cdot \nabla)$$

And finish up by assuming plane monochromatic field for  $\mathbf{A}$ , expanding the exponential again, and evaluating  $\nabla$  by setting

$$-2i\hbar\mathbf{p} = 2m[\mathcal{H}^0, \mathbf{r}]$$

Get expressions for the transition rates equal to the classical ones, multiplied by a dimensionless factor, the 'oscillator strength'  $f$ . For absorption  $|i\rangle$  to  $|f\rangle$ , for instance (electric dipole term, averaged over polarization):

$$f_{i \rightarrow f} = \frac{2}{3} \frac{m\omega_{if}}{\hbar} |\langle f | \mathbf{r} | i \rangle|^2$$

Note that the matrix element  $\langle f | \mathbf{r} | i \rangle$  brings in the **selection rules** for transitions between states. Electric dipole **forbidden transitions** have  $\langle f | \mathbf{r} | i \rangle = 0$ ; but the transition may still occur in higher-order multipole terms (E2, M1, ...).

**So now we have the basics of atomic structure, and the means to evaluate radiative transition probabilities. Once again, I urge you to read Steve Kahn's review for more details. Remember, a lot of Astro-H spectroscopy will be for heavy ions (high-Z): relativistic and higher order processes important!**

# Excitation Processes

In most astrophysical plasmas of interest to us<sup>(\*)</sup>, **electron densities are very low-**

collisional downward transition rate between two levels typically much smaller than radiative (spontaneous) decay rate:

$$n_e C_{21} \ll A_{21} \quad (A_{21} \text{ large for X-ray transitions!})$$

so that most of the time, excitation of an ion is followed by photon emission; electron thermal energy goes into excitation, but excitation does not return energy to the thermal energy pool.

the excited state populations are near-zero: excitation balance is very far from thermodynamic equilibrium.

Critical density:  $n_e \sim A_{21}/C_{21}$ . For higher  $n_e$ , ions start to go into T.E.

In addition: **radiation energy densities  $\ll$  blackbody** (because  $\tau \ll 1$ ), so radiative excitation and induced emission not important (with one exception: resonance lines)

*(convince yourself with the 2-level atom!)*

(\*) excluding stellar interiors and atmospheres, accretion flows, ...

Processes that populate excited states:

- (1) collisions with charged particles (collisional excitation, CX)
- (2) absorption of a photon (photoexcitation)
- (3) recombination ion-free electron into excited state  
(radiative or dielectronic recombination [RR, DR]; 3-body processes)
- (4) charge exchange processes (CX)
- (5) 'innershell ionization'

## (1) Collisional excitation

mostly electron-ion collisions; proton collisions rarely important (shocks?)

cross section: **very roughly of order (electron de Broglie wavelength)<sup>2</sup>:**

$$Q_{ij}(v) = \frac{\pi}{w_i} \left( \frac{\hbar}{p} \right)^2 \Omega_{ij} \quad (\text{cm}^2)$$

( $w_i$ : statistical weight lower state;  $p$ : momentum of free electron;  
 $\Omega$ : 'collision strength', of order unity)

**Also very roughly of order 'geometric' cross section of ion:**

$$Q_{ij}(U) = \frac{\pi a_0^2}{w_i} \frac{\mathcal{R}}{E_{ij}} \frac{\Omega(U)}{U} \quad (\text{cm}^2)$$

( $U = E/E_{ij}$ ;  $E$  electron energy;  $a_0$ : Bohr radius;  $\mathcal{R}$ : Rydberg energy).  
To see this: set  $E_{ij} \sim Z^2 \mathcal{R}$ ; recall: radius of first Bohr orbit in H-like ion of nuclear charge  $Z$ :  $r_1 = a_0/Z$ .

Convenient parameterizations of  $\Omega(U)$ : start with Kaastra *et al.* (see bibliography)

In thermal plasma of electron temperature  $T_e$ , the total rate averaged ( $\langle \dots \rangle$ ) over the electron thermal energy distribution:

$$S_{ij} = n_e n_i \langle Q_{ij} v \rangle = 8.62 \times 10^{-12} \langle \Omega(y) \rangle w_i^{-1} T^{-1/2} e^{-y} \text{ m}^{-3} \text{ s}^{-1}$$
$$8.62 \times 10^{-18} \text{ cm}^{-3} \text{ s}^{-1}$$

$$y = E_{ij}/kT_e$$

Only electrons with  $E > E_{ij}$  contribute, so in thermal plasma, excitation rate depends exponentially on  $E_{ij}/kT_e$

NB: the above generally applies to permitted transitions. For forbidden transitions, the cross section and rates depend differently on  $E$  and  $T$ .

(2) photoabsorption: see Jelle Kaastra's lectures.

As an excitation mechanism, important only in very specific cases: scattering of external continuum photons by resonance transitions(\*); scattering of resonance line photons.

(3) Recombination: Radiative, dielectronic, 3-body.

**Radiative recombination (RR):** inverse of photoionization.

Consider Thermodynamic Equilibrium (TE): in TE, RR and PI rates balance.

Resulting relation between cross sections: the Milne Relation.

Inserting photoelectric absorption cross section, averaging over

Maxwell distribution:

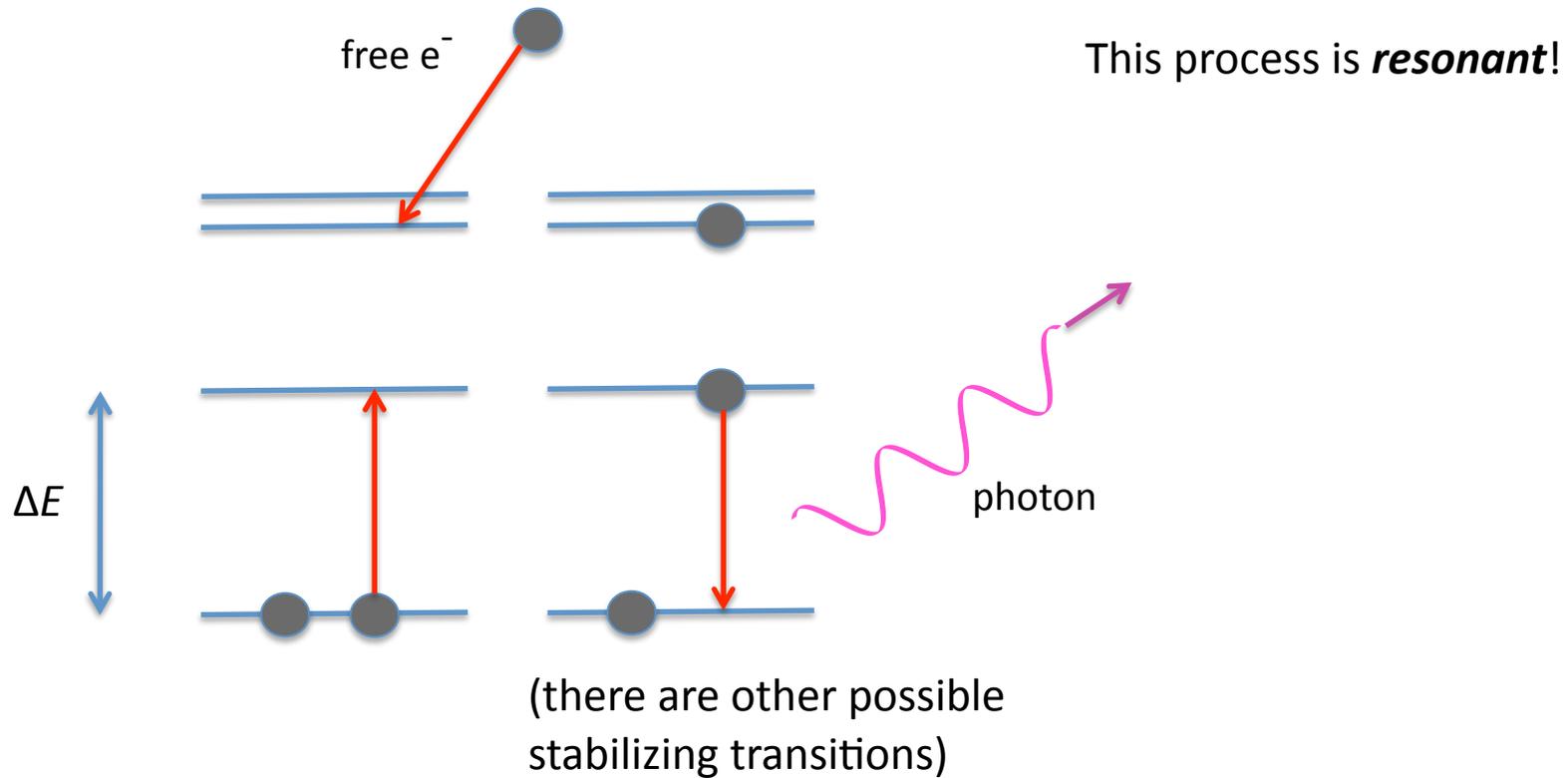
low temperatures ( $kT \ll$  ionization potential):  $R \sim T^{-1/2}$

high temperatures ( $kT \gg$  ionization potential):  $R \sim \ln(\chi/kT) T^{-3/2}$

so recombination effective at low temperatures.

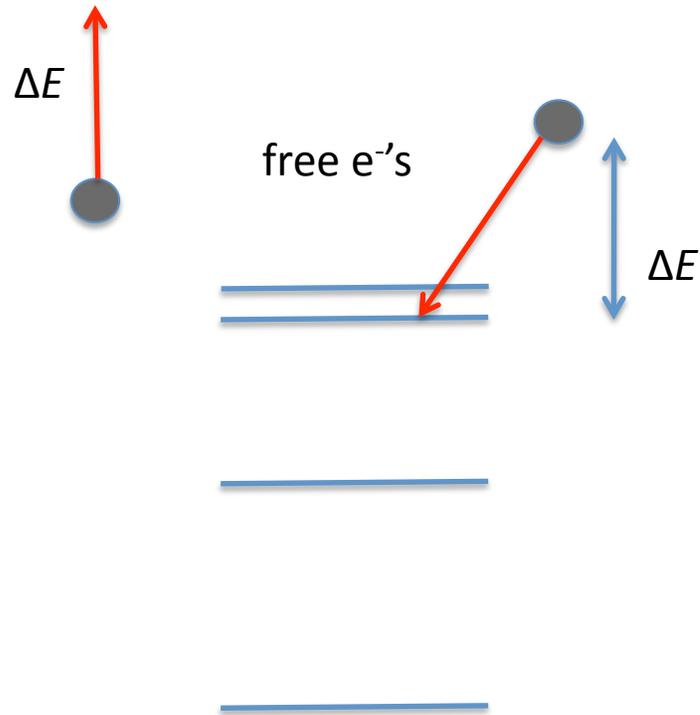
(\*) resonance transition: lowest-energy transition from the ground state, so  $n=1-2$

## Dielectronic recombination (DR):



DR is often more important than RR; note that at low temperatures, such that  $kT \ll \Delta E$ , DR is suppressed (free electron needs to excite bound electron)

### 3-body recombination: inverse of collisional ionization



Rate proportional to  $n_e^2$ , so only important at high densities.

All recombination processes can leave ion in excited state, and produce photon(s)  
Recombination tends to populate different excited states than CX:  
resulting spectrum different from collisional spectrum.

#### (4) Charge exchange (CX)

Two ions exchange bound electron; in astrophysical case, collisions of heavy ions with H and He-ions vastly outnumber other combinations.

Practical example: highly charged Oxygen ion plus H atom: leaves

Oxygen one charge state lower, in excited state, plus a proton.

Occurs for instance when solar wind (highly ionized) collides with Geocorona.

Should also occur near astrophysical shocks moving into near-neutral medium.

Again, the process tends to excite to different levels than CX: causes characteristic emission spectrum.

#### (5) Innershell processes

Free electron, photon, or cosmic ray removes  $n=1$  or  $n=2$  electron from atom or ion:  
ion stabilizes via emission of electron (Auger process) or photons (“fluorescence”)

Examples: irradiated neutral gas; ionizing transient plasmas (SNR).

Important for Astro-H: Fe has high fluorescence yield;

Fe K band first time at high resolution with Astro-H.

# Ionization balance

We already discussed recombination processes; briefly discuss ionization processes and ionization balance.

Collisional ionization: very similar to CX; see page 18.

Photoionization: 'photoelectric absorption' liberates electron; textbook calculation (Compton ionization; see Kaastra *et al.*)

Either process can eject a valence electron, or an innershell electron; the latter case can be complicated: Auger process can result in emission of multiple electrons; ion changes charge state by several steps at once.

Calculate the ionization balance:

$$dn_i/dt = +(\text{all ionizations from lower ions}) - (\text{all ionizations to higher states}) + (\text{all recombinations from higher states}) - (\text{all recombinations to lower states});$$

the terms in brackets are the relevant rates of change of  $n_i$ , in  $\text{cm}^{-3} \text{sec}^{-1}$ .

Set of ***coupled linear equations*** (matrix equation) for the ions of a given element.

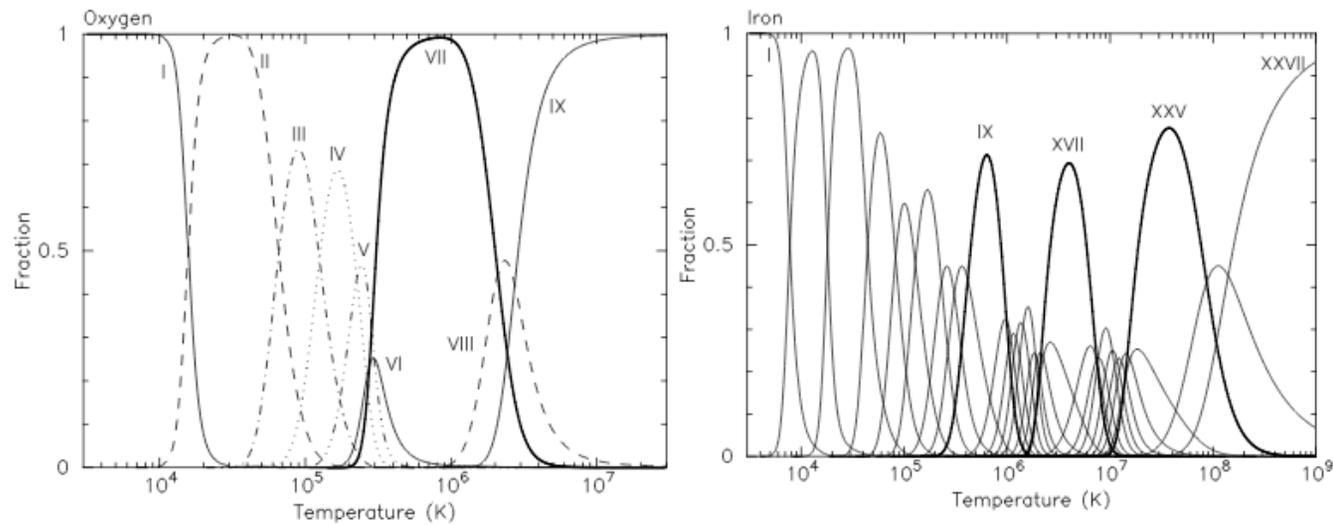
Equilibrium: all  $dn_i/dt = 0$

Common types of equilibrium:

balance between collisional ionization and RR+DR:

**collisional ionization equilibrium (CIE)**, a.k.a. “hot gas”

since all rates only depend on  $T$ , balance fully determined by  $T$  alone.



**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.

From Kaastra *et al.*

**Photoionization equilibrium:** balance between photoionization and RR+DR

Consider equilibrium between two charge states,  $i$  and  $i+1$ :

$$n_i \int_{\chi}^{\infty} \frac{F_{\nu}}{h\nu} \sigma_{\nu} d\nu = n_e n_{i+1} \alpha(T_e)$$

$F$ : incident radiation flux  
 $\sigma$ : photoelectric cross section  
 $\alpha$ : total recombination coeff.  
 $\chi$ : ionization potential  $i, i+1$

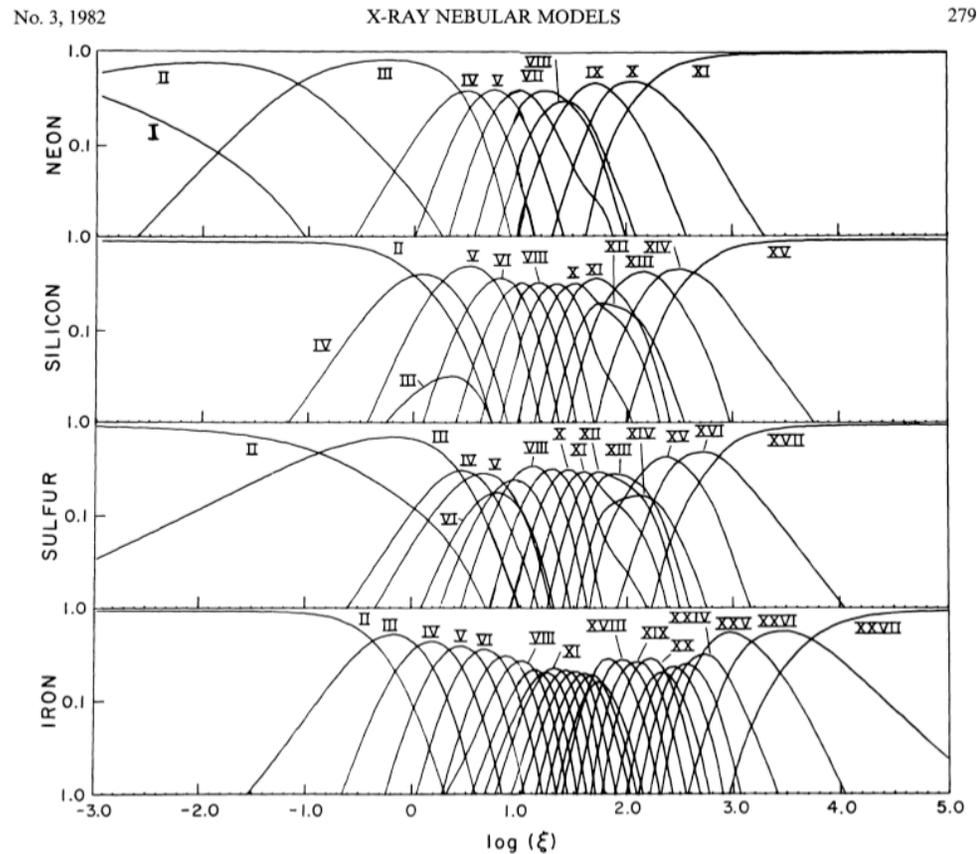
so

$$\frac{n_{i+1}}{n_i} = \frac{\int_{\chi}^{\infty} \frac{F_{\nu}}{h\nu} \sigma_{\nu} d\nu}{n_e \alpha(T_e)} = \frac{F}{n_e} \times \frac{\int_{\chi}^{\infty} \frac{f_{\nu}}{h\nu} \sigma_{\nu} d\nu}{\alpha(T_e)} \quad (F_{\nu} = F \cdot f_{\nu})$$

The ionization equilibrium only depends on ratio  $\xi = F/n_e$ : the *ionization parameter*(\*); the second factor can be calculated for given spectrum and cross section, once and for all.

(\*) alternative definitions are also current

- (1) Note that thermal balance and ionization balance are coupled
- (2) Since ionization produced by photons, no requirement that  $kT_e \sim$  characteristic ionization potentials,  $\chi$ . In fact, photoionized plasmas typically equilibrate at  $kT_e \sim 0.1 \chi$  (photoionized gas is cool).
- (3) Photoionization balance typically 'messier' than collisional case: Maxwell distribution of  $e^-$  energies is sharply peaked at  $(3/2) kT_e$ , but typical photoionizing spectrum is very broad in photon energy.



Kallman & McCray,  
*ApJS*, **50**, 263 (1982)

Which type of equilibrium prevails?

Compare the collisional and photoionization timescales:

$$\tau_{\text{photo}}^{-1} = F \int_{\chi}^{\infty} \frac{f_{\nu}}{h\nu} \sigma_{\nu} d\nu$$

$$\tau_{\text{collisional}}^{-1} = n_e C_{i,i+1}(T_e)$$

$C_{i,i+1}$ : collisional rate coefficient

$$\frac{\tau_{\text{photo}}}{\tau_{\text{collisional}}} = \frac{n_e C_{i,i+1}(T_e)}{F \int_{\chi}^{\infty} \frac{f_{\nu}}{h\nu} \sigma_{\nu} d\nu}$$

> 1 : collisional ionization

< 1 : photoionization

So for **low density**, high radiation intensity plasmas, photoionization prevails;

Otherwise: collisional ionization dominates.

And of course, a mixture is also possible (the IGM?)

## And now we also have the concepts to describe non-equilibrium situations:

Compare the 'age',  $\tau$ , of your plasma to  $\tau_{\text{collisional}}$  or  $\tau_{\text{photo}}$  !

If  $\tau < \tau_{\text{collisional}}$  or  $\tau_{\text{photo}}$  , your plasma is still ionizing (SNR, solar flares, IGM, ...)

Similar considerations applied to the recombination timescales (recall, photoionized gas usually much cooler than collisionally ionized gas, so relevant recombination rate coefficients may be very different) tells you whether your plasma may be recombining.

Example:

'NEI', non-equilibrium ionization (conventionally applied to collisional plasmas only) (simplify to two ionization states):

$$dn_i/dt = + n_e n_j C_{j,i+1} - n_e n_{i+1} \alpha_{i+1,i}$$

$$dn_i/d(n_e t) = + n_j C_{j,i+1} - n_{i+1} \alpha_{i+1,i}$$

So time development controlled by  $n_e t$  (also referred to as the 'ionization parameter', confusingly). Generally, when  $n_e t > 10^{11-12} \text{ cm}^{-3} \text{ s}$ , ionization has equilibrated—'old' and high-density plasmas.

# apology

We only have an hour, so you won't find data and numbers here for the various physical quantities we discussed (cross sections, rate coefficients, wavelengths, ...).

All of these are implicit in the various codes Randall will discuss, so you're fine(\*).

But if you want a cross section, or a rate coefficient, to do some calculations and estimates (*rather than blindly fit*), the next slide gives good starting points. For accurate numbers, search the literature.

(\* ) *do remember that you may encounter spectra that reveal inaccuracy or inadequacy in those numbers!! Science is hard!!*

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(2) Typo in definition of  $U$  (at his Eq.(1))

(3) Online at <http://www.springerlink.com/content/x42xp7fxv2fm/>

