Emission mechanisms
Part II

Some reference textbooks:

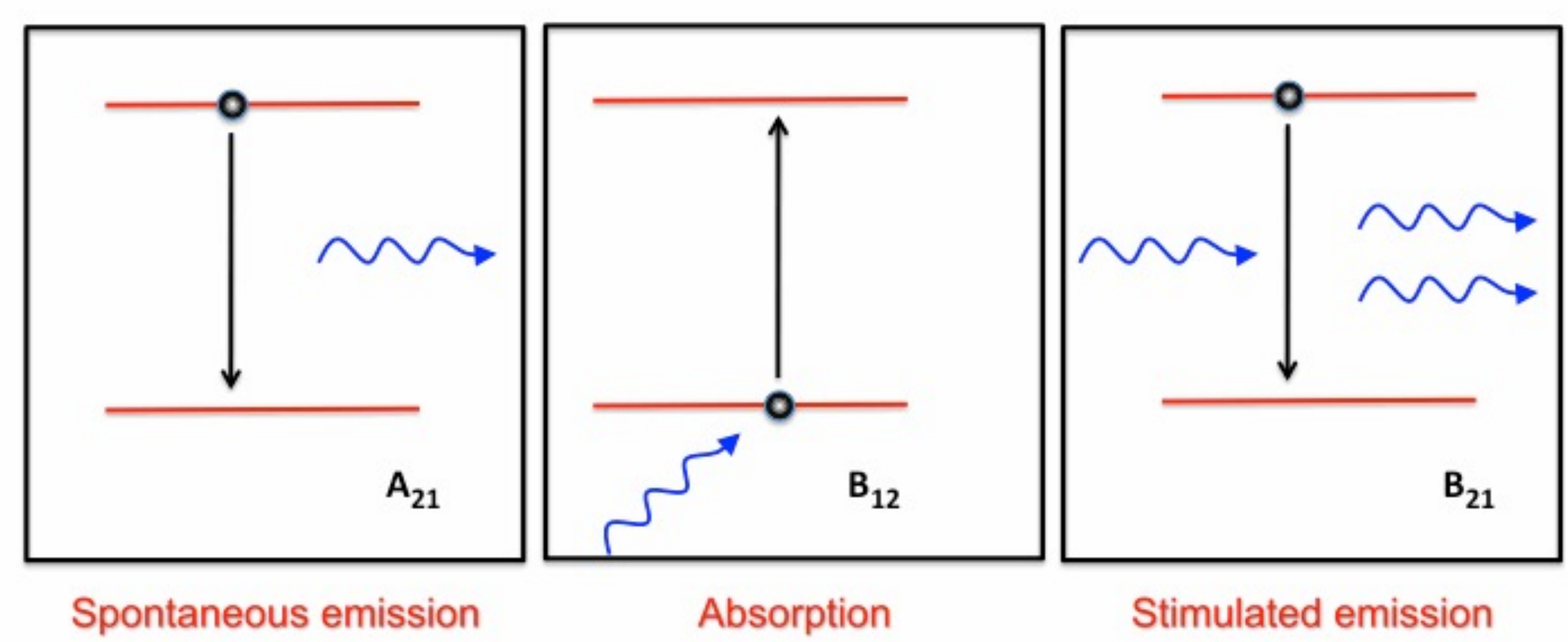
- Bradt, *"Astrophysics Processes", Cambridge University Press*
- Rybicki & Lightman*, "Radiative processes in astrophysics", Wiley*
- Ghisellini*, "Radiative processes in High-Energy Astrophysics"* (arXiv:1202.5949) & Lecture Notes in Physics 873 (Springer)
- Kahn et al., "*High-Energy Spectroscopic Astrophysics*", Springer
- Pradhan & Nahar, "Atomic Astrophysics and Spectroscopy", Cambridge University Press

Outline of part II

- Basics on atomic transitions: Einstein’s coefficients.
- Line profile and broadening, curve of growth
- Photon and collisional excitation/de-excitation
- Ionization/recombination processes
- Collisional equilibrium − Cooling via line emission
- Photoionization equilibrium

Einstein's coefficients (for atoms). I

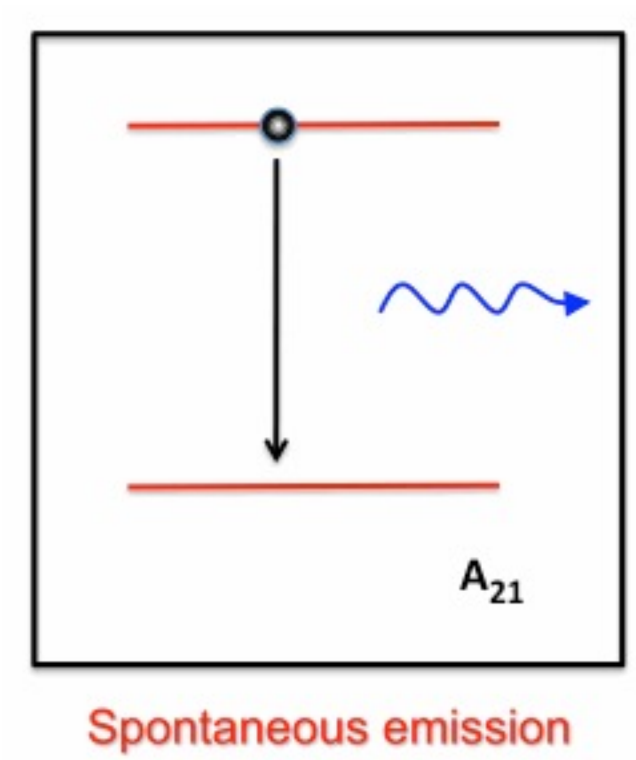
Einstein's coefficients concern the probability that a particle spontaneously emits a photon, the probability to absorb a photon, and the probability to emit a photon under the influence of another incoming photon. Valid for all radiation fields

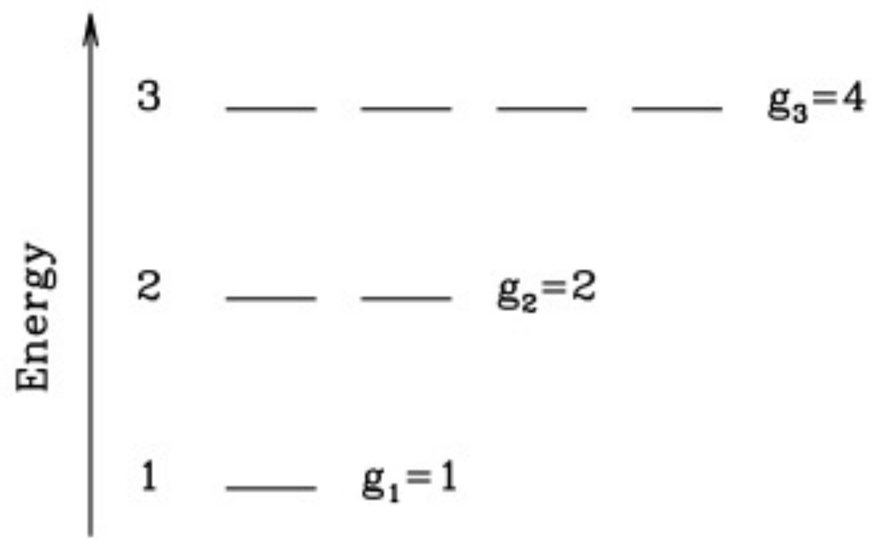


Einstein's coefficients. II

➢ **Spontaneous emission**. The system is in an excited level 2 at energy $E+h\nu_0$ and drops to a lower level 1 (energy E) by emitting a photon of energy $h\nu_0$

A_{21}: transition probability per unit time of spontaneous emission [s^{-1}]





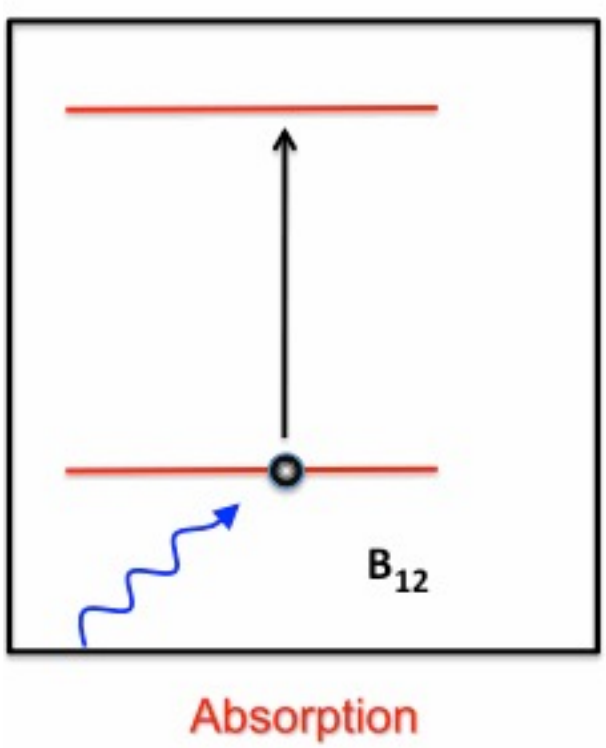
Energy levels with weights

Einstein's coefficients. III

- **Absorption**. The system, at level 1 with energy *E*, absorbs a photon of energy $h\nu_0$ and reach the level 2 at energy $E+h\nu_0$. The transition probability depends on the radiation field.

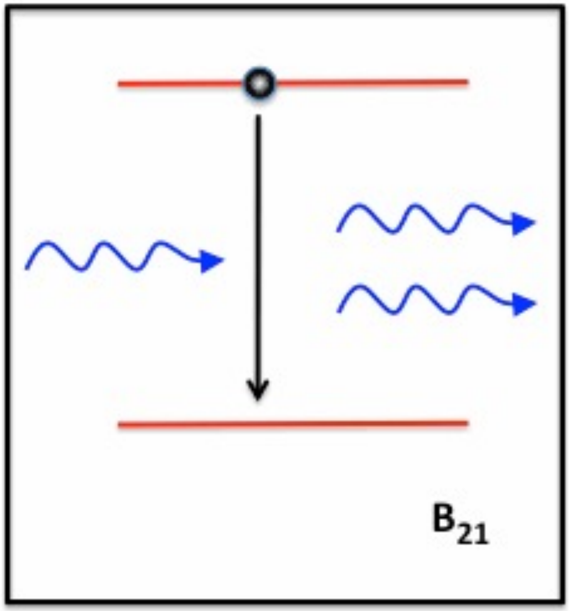
$B_{12}J$: transition probability of absorption per unit time

J=J_ν=intensity of the radiation field $$J_\nu = \frac{1}{4\pi}\int I_\nu d\nu$$



Einstein's coefficients. IV

➢ **Stimulated emission**. The system goes from level 2 to level 1 stimulated by the presence of a radiation field ($h\nu_0$ corresponding to the energy difference between levels 2 and 1).
The energy of the emitted photon is the same as of the incoming photon (also direction and phase are the same → coherent emission: laser, maser…)
$B_{21}J$: transition probability of stimulated emission per unit time



Stimulated emission

Einstein's coefficients. V

At the equilibrium, the rate of emission must be equal to the rate of absorption

Transitions 1 ➔ 2 equal to Transitions 2 ➔ 1
n_1,n_2: number density of e^- in levels 1,2

$$n_1 B_{12} J_v = n_2 A_{21} + n_2 B_{21} J_v$$

$$J_v = \frac{A_{21}/B_{21}}{(n_1/n_2)(B_{12}/B_{21}) - 1}$$

Thermodynamic equilibrium (Boltzmann): J=B(T)

$$\frac{n_1}{n_2} = \frac{g_1}{g_2}\frac{e^{-E/kT}}{e^{-(E+hv)/kT}} = \frac{g_1}{g_2} e^{h\upsilon_{21}/kT}$$

Statistical weights g_j: degeneracy of a state, i.e., number of sub-states (e.g., n=1 ➔ 2 (2 s states); n=2 ➔ 8, 2 s and 6 p states)
The ratio g_j/g_i tells us the probability of a state being proportional to its statistical weight

$$\Rightarrow J_\nu = \frac{A_{21}}{B_{21}\left[\left(\frac{g_1 B_{12}}{g_2 B_{21}}\right)e^{\frac{h\nu_{21}}{kT}} - 1\right]}$$

Equilibrium: J_ν=black body intensity

$$g_1 B_{12} = g_2 B_{21}$$

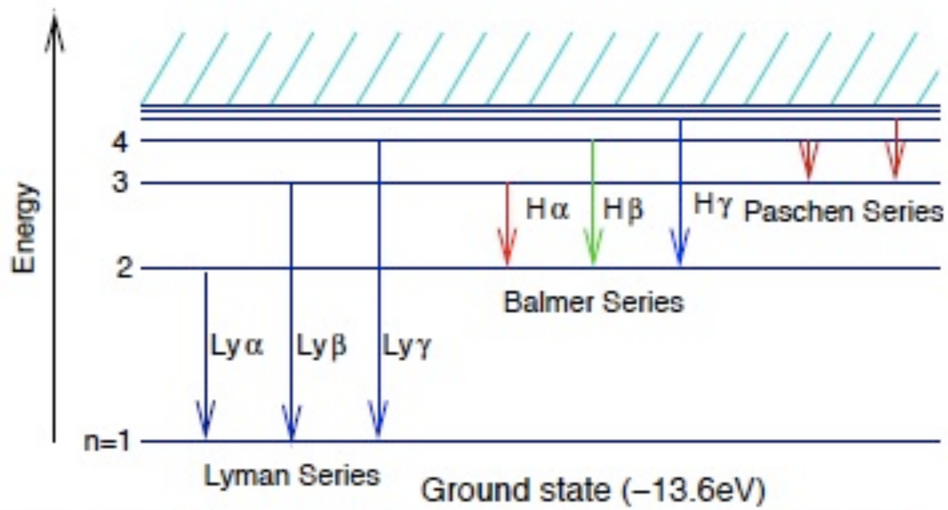
$$A_{21} = \frac{2h\nu_{21}^3 B_{21}}{c^2}$$

called "detailed balance relations" and valid universally (not only for thermodynamic equilibrium), independent on T

Not all atomic transitions are allowed. Selection rules are such that *ΔS=0, ΔL=0,±1, ΔJ=0,±1* (but *J=0 → 0 strictly forbidden*).
S=spin angular momentum; L: orbital angular momentum; J=total angular momentum
However, selection rules may be violated because they are derived in an approximated way. In practice, strictly forbidden means very low probability of occurrence

Bohr-Sommerfeld Theory – Energy levels

Bohr-Sommerfeld Theory



Line emission through transitions between orbits with different n. Photon energy:

$$h\nu_{21} = \frac{2\pi^2 \mu e^4 Z^2}{\hbar^2} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \tag{9.10}$$

where the constant is called 1 Rydberg:

$$1\,\text{Ry} := \frac{2\pi^2 \mu e^4}{\hbar^2} \sim 13.6\,\text{eV} \tag{9.11}$$

Line profile – Natural broadening

Underlying statement: all the spectral lines have a finite width and a particular profile. Width and shape of a line depend directly in atomic transitions and plasma environment

Let us call $\varphi(\nu)$ the probability that the transition occurs by emitting or absorbing a photon with energy $h\nu$ (*emission or absorption line* $(\int\varphi(\nu)d\nu \equiv 1)$). An unavoidable source of broadening is due to the *uncertainty principle* – $dE\, dt \geq h/2\pi$, dt being the timescale of decay (finite lifetime of energy levels)

This natural broadening has the form of a *Lorentzian function* (γ is the decay rate, damping constant) ➔ *damping profile*

$$\phi(\nu) = \frac{\gamma/4\pi^2}{(\nu-\nu_0)^2 + (\gamma/4\pi^2)}$$

γ= FWHM of the line profile, proportional to the transition probability
ν_0=central frequency of the line

Damping profile (damping term of the classical oscillator)

The longer the atom is in a state (**dt** high), the more precisely its energy can be measured (**dE** low)

A large *transition probability* leads to a short life in the state (low *dt*) and a large energy uncertainty (high *dE*)

Line profile – Thermal broadening

Thermal broadening: the atoms in the gas will have a thermal spectrum governed by the Maxwell-Boltzmann velocity distribution.
Radiation emitted or absorbed by the atoms receding/approaching the observer will be shifted in frequency

Natural + thermal broadening → ***Voigt profile***, composed by a **Doppler core** and **Lorentzian wings**

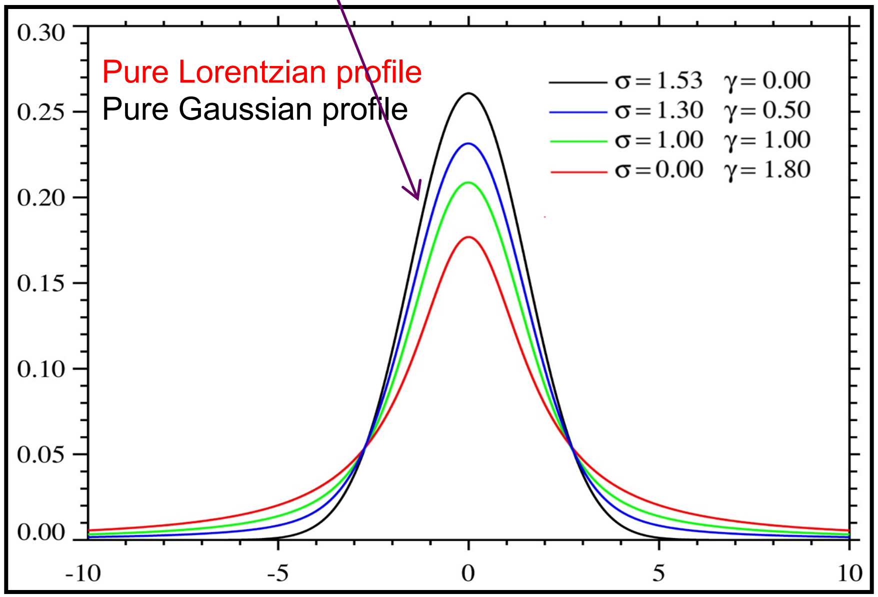
$$\phi(\nu) = \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{(\nu-\nu_0)^2}{\sigma^2}}$$

$$\sigma = \frac{\nu_0}{c}\sqrt{\frac{2kT}{m}}$$

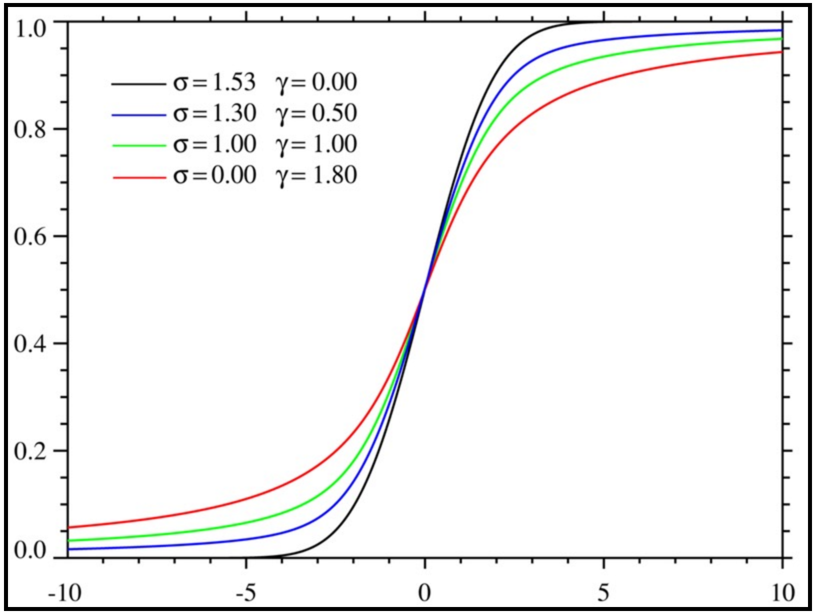
Doppler (thermal) broadening profile

$$\sigma = \frac{\nu_0}{c}\sqrt{\frac{2kT}{m} + \zeta}$$

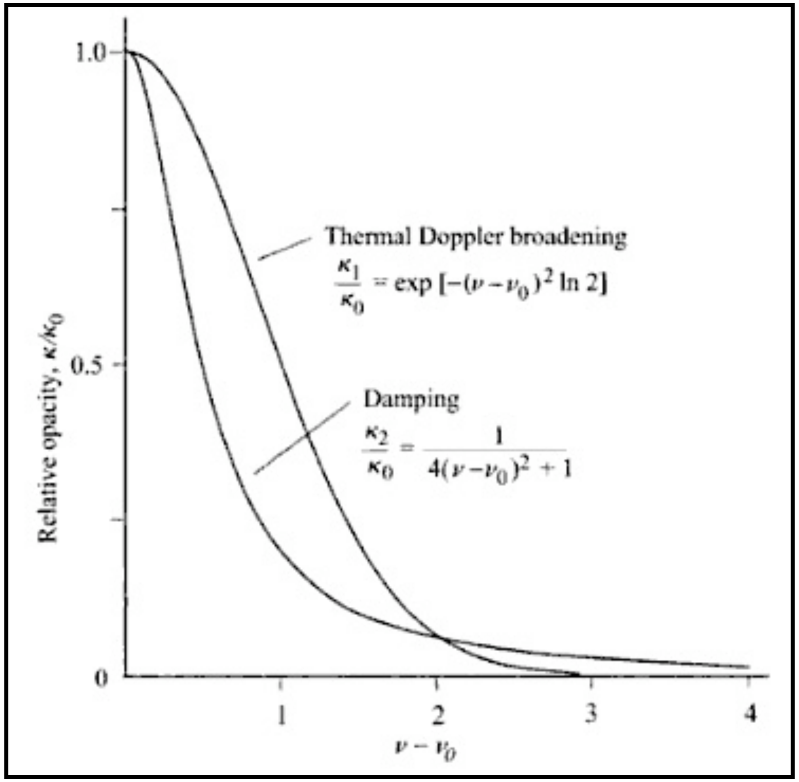
In case of microturbolence



Probability density function



Cumulative probability distribution



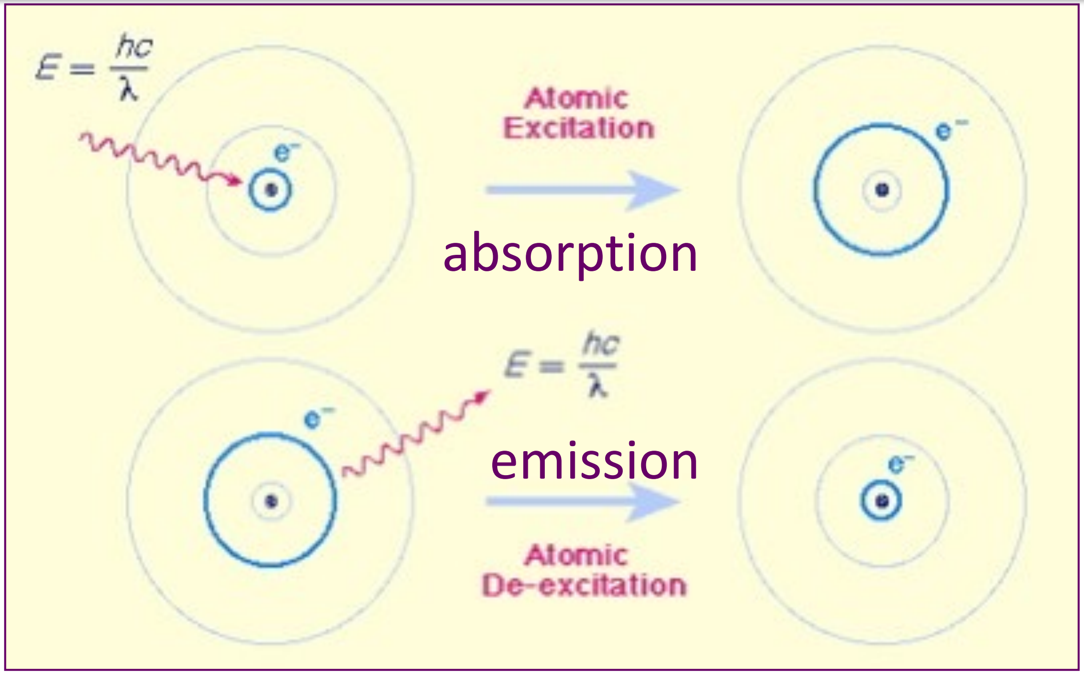
The **Gaussian** component dominates the line core (or is confined to it), while the **Lorentzian** profile dominates in the line wings out to several times the FWHM

Additional line broadening mechanisms:

• Doppler broadening by rapid motions of clouds emitting/absorbing photons (*bulk turbolent motion*). The velocities of the clouds are not necessarily thermally distributed.

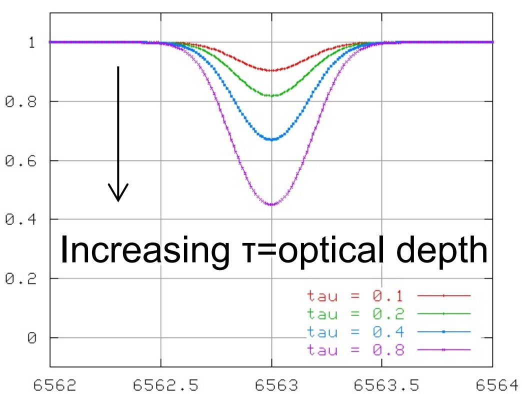
• *Collisional (pressure) broadening*: collisions in the gas de-excite atoms before they naturally decay, thus changing the damping profile (measure of the number of collisions, hence of the density of the gas).

Photon excitation/de-excitation



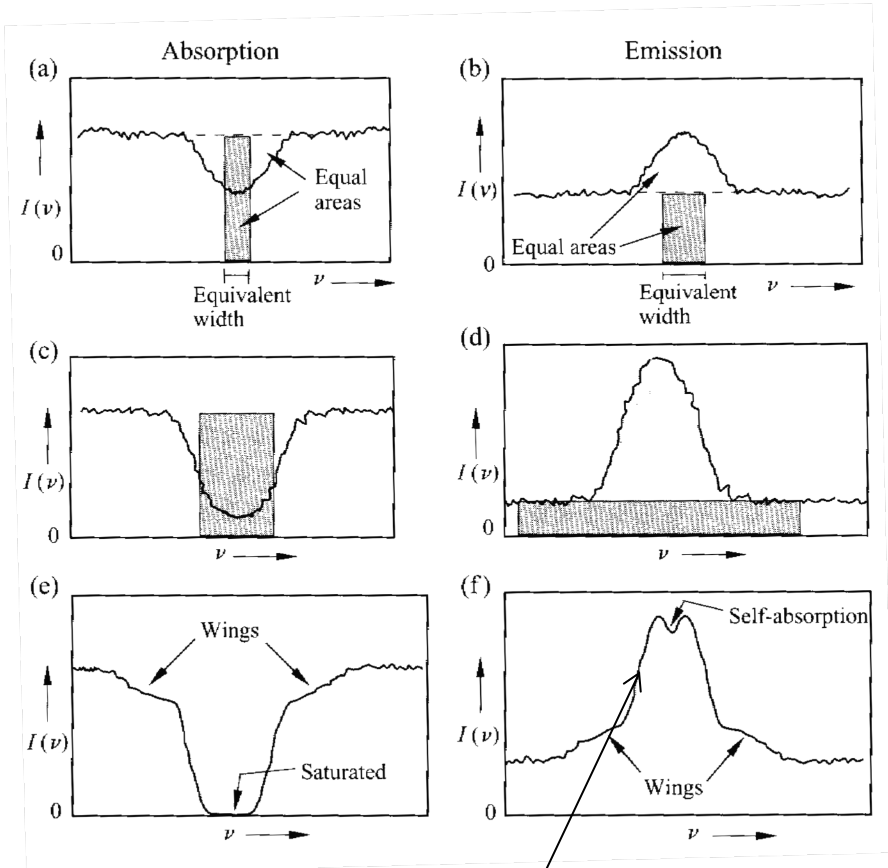
A photon can be absorbed by an electron in an atom, which jumps to a higher level (***excitation***). The probability of absorption depends on the *oscillator strength f* (related to the Einstein coefficients).
f is a measure of the intrinsic strength of an atomic transition and intensity of a spectral line.
f is large for *resonant lines*, low for *forbidden lines.*
Bound-state transition

$$EW = \int \frac{I_\nu(c) - I_\nu(l)}{I_\nu(c)} d\nu$$



Line absorption (emission) from a population of atoms is measured in terms of *Equivalent Width (EW).*
$I_\nu(c)$: intensity of the continuum without absorption (emission)
$I_\nu(l)$: actual intensity of the continuum in presence of the line
It corresponds to the area in the spectrum removed by e.g. the absorption, and depends on the probability of the transition and the amount of matter.

Large EW → the line is "pronounced" compared to the continuum flux

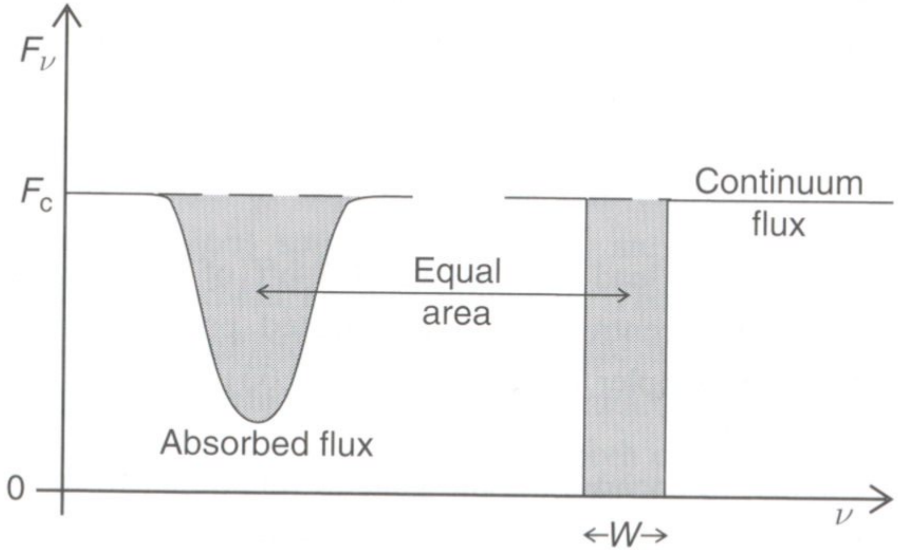


Weak lines

Strong lines

Lines with broad (pressure-broadened) wings and self-absorption

The emitting cloud can absorb its own radiation (often observed in AGN optical spectra, e.g., in $CIV_{1549Å}$)



$$EW = \int \frac{F_C - F_\nu}{F_C} d\nu$$

F_C : measured continuum intensity

F_ν : measured line intensity

at a given frequency

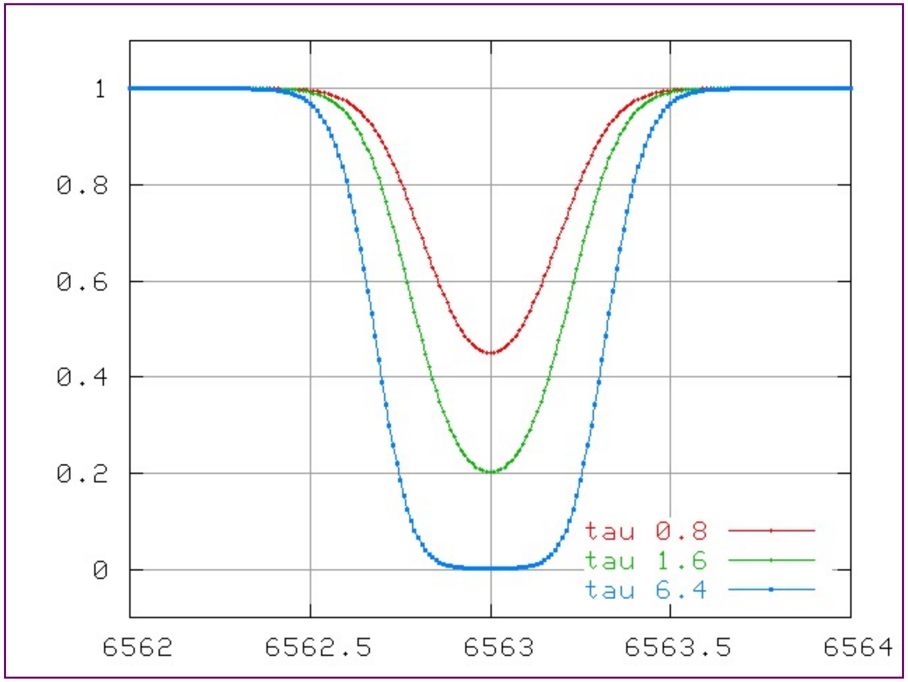
EW is related to the number of ions producing the line and the strength of the transition

$$\frac{F_\nu}{F_C} = e^{-\tau_\nu} \rightarrow EW = \frac{\lambda^2}{c}\int (1 - e^{-\tau_\nu})\, d\upsilon \xrightarrow{\tau << 1 \text{(ISM)}} \frac{\lambda^2}{c}\int \tau_\upsilon\, d\upsilon$$

$$\tau_\upsilon = \left(\frac{\pi e^2}{m_e c^2}\right) \mathrm{N_i}\ \mathrm{f}_\upsilon\ \phi(\upsilon)$$

$$\mathrm{EW} = \left(\frac{\pi e^2}{m_e c^2}\right) \mathrm{N_i}\ \mathrm{f}_\lambda\ \lambda^2$$

N_i=number of absorbers
f=oscillator strength
Φ(v)=line profile



If matter is optically thin even at the line center, the line profile is unsaturated at any frequency. Increasing the optical depth, the line saturates, first in the Doppler core and then in the Lorentzian wings

Curve of growth: EW=f(N_H)

Optically thick in the wings: the weak wings due to collisional broadening become important: damped profile

EW prop $N^{1/2}$

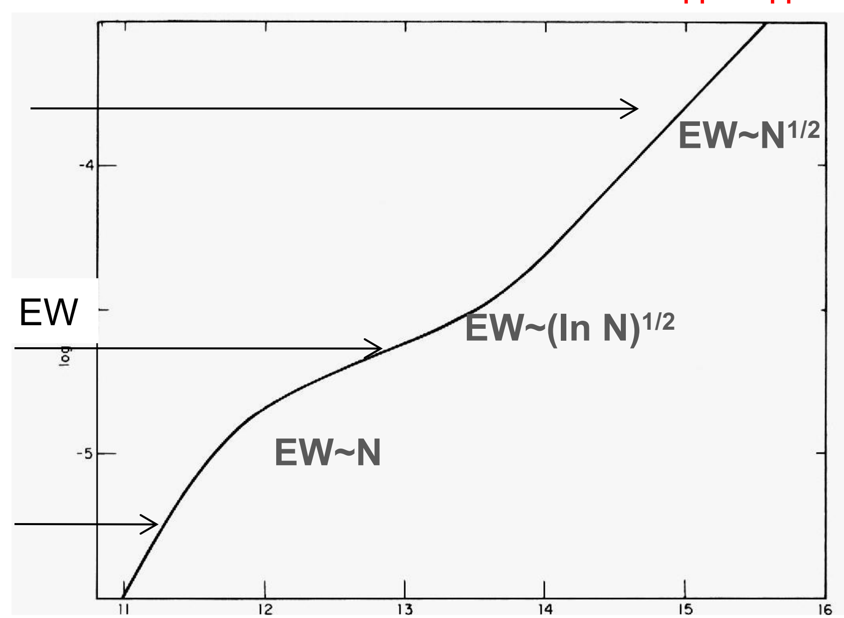
Optically thick in the core: low-velocity atoms completely absorb the photons near the central ν. *The line saturates*: more atoms increase slightly EW

EW prop $(\ln N)^{1/2}$

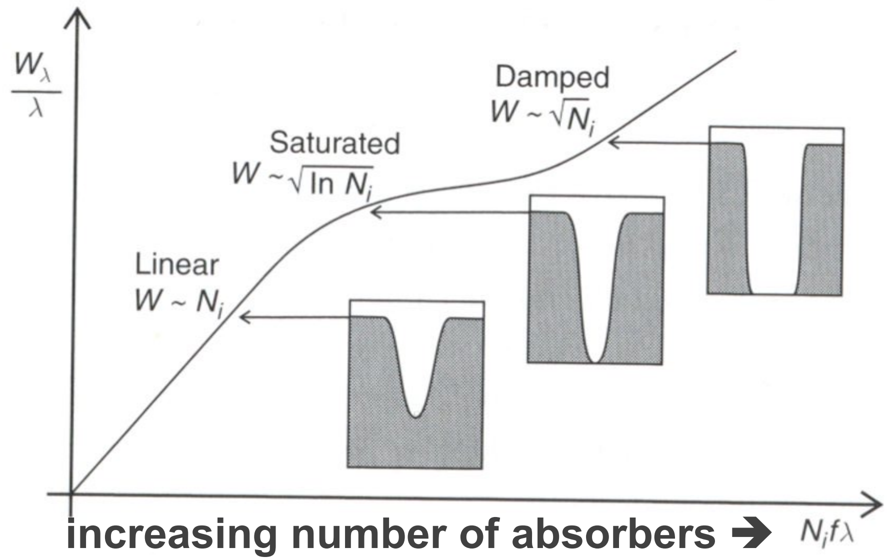
Optically thin: the atoms along the l.o.s. are few and block only a small portion of the beam.

EW prop N

$N_H = n_H R$



Number of absorbing atoms along the l.o.s.



EW as a function of temperature and density:
Curve of Growth

The deepeening and broadening of the line are proportional to the energy removed from the continuum by an increasing number of absorbers

$$EW/\lambda = \left(\frac{\pi e^2}{m_e c^2}\right) N_i \, f_\lambda \, \lambda$$

Linear part: $EW \sim N_i$, optically thin regime

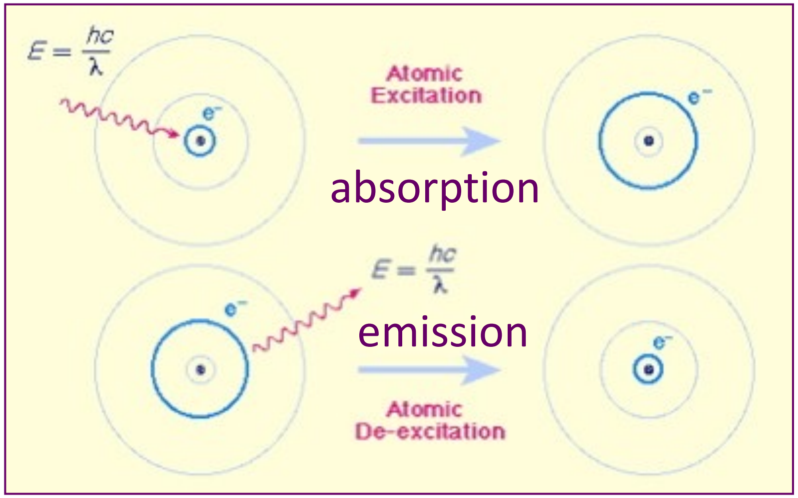
$$EW \sim \sqrt{\ln N_i}$$

Saturated part: the density of the ions is sufficient to absorb nearly all of the continuum photons at the line central wavelength

$$EW \sim \sqrt{N_i}$$

Damped part: ions absorb photons in the line wings, which are then seen to be 'damped' beyond the line center ('square' shape)

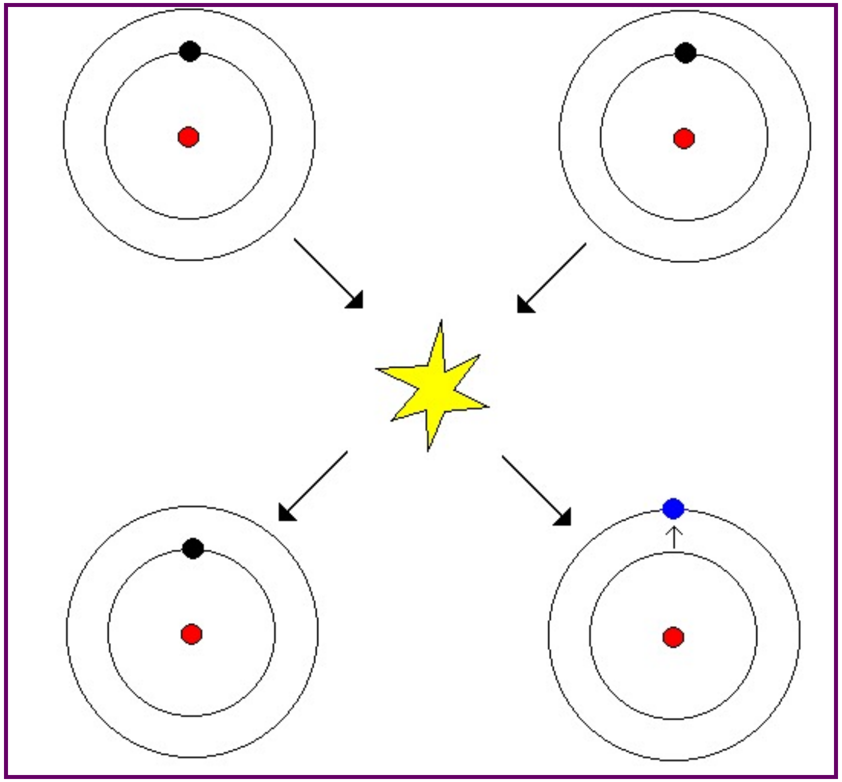
The inverse process to excitation is **de-excitation**, when an electron in an excited level falls into a lower level by emitting one (or more, if the de-excitation occurs as a cascade) photon. Also for the emission lines can be defined an equivalent width with the same definition as before (the sign of the EW is the opposite)



If line emission occurs via the exact inverse transition with respect to absorption, the process is called *resonant scattering*. Resonant scattering is important for resonant lines, both because absorption is more likely (larger oscillator strengths) and because forbidden de-excitation occurs on long timescale (and therefore something different is likely to occur in the meantime).

In resonant scattering, the frequency of the incoming photon is close to the frequency of an energy transition of a bound electron in an atom or molecule ➔ the electron responds in resonance with the radiation

Collisional excitation/de-excitation



An atom can be excited by interacting with another atom or a free electron.

The inverse process is **collisional de-excitation**, when an electron in an excited atom falls to a lower level providing the energy to the passing electron.

Ionization/recombination

Process (ionization)	**Inverse process (recombination)**
Collisional ionization	3-body recombination
Photoionization (Photoelectric absorption)	Radiative recombination
Autoionization (Auger effect)	Dielectronic recombination

Ionization/recombination in a nutshell

Collisional ionization: similar to collisional excitation, but the excited electron ends up in a continuum, rather than a bound state.

3-body recombination: 2 free electrons interact with an ion. One of them gets captured, the other one remains free, carrying out the excess energy.

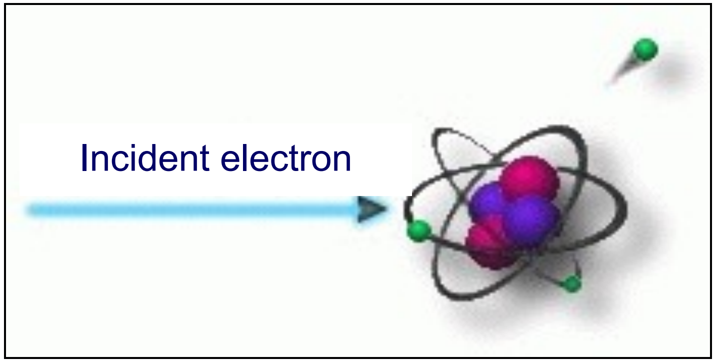
Photoionization: a bound electron is ejected from the atom by the absorption of a photon with an energy larger than the ionization potential.

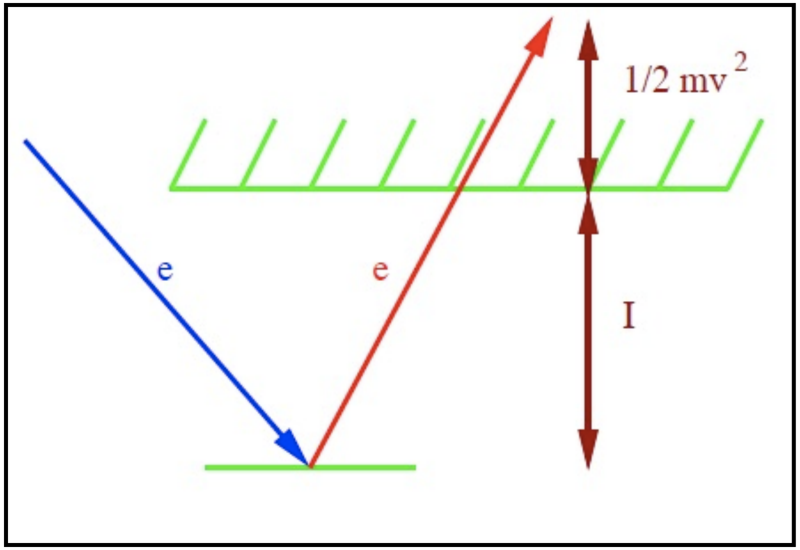
Radiative recombination: capture of a free electron by an atom with release of one or more photons (cascade).

Autoionization (Auger effect): an excited atom decays by ejecting an electron from an outer levels (see also fluorescence emission).

Dielectronic recombination: capture of a free electron, with the excess energy used to excite the atom. The excited atom may then decay radiatively.

Collisional ionization



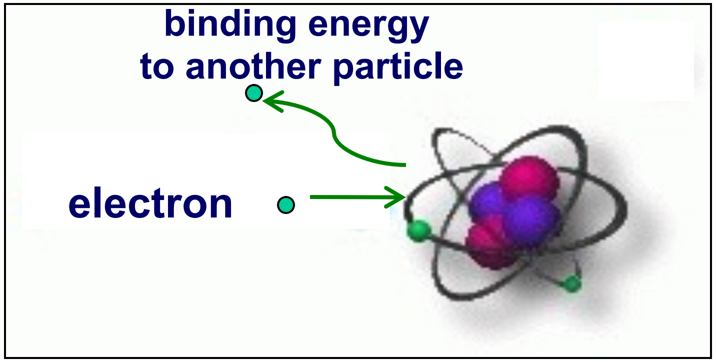


Collisional ionization is the process whereby a free electron strikes an ion, with sufficient energy to strip out an electron. An energy equal to the ionization potential of the atom (13.6 eV in the case of hydrogen) is removed from the incoming electron.

Collisional ionization is therefore a process which cools the electron gas.

It is the inverse process of three-body recombination.

3-body recombination

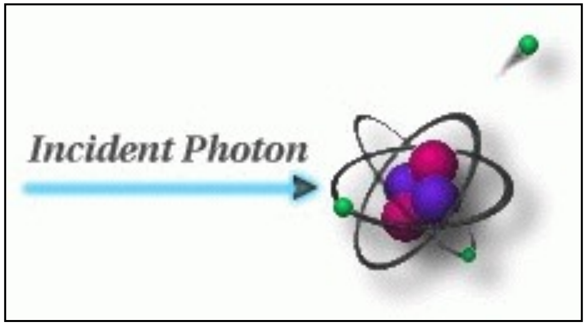


In the 3-body recombination, a free electron with a given velocity is captured by an atom or ion into a bound state (*free-bound emission*).

The excess (binding) energy is transferred to a third particle (in general, an electron), which also takes care of momentum conservation.

The 3-body recombination, where no radiation is emitted, becomes significant in high-density environments (large number of particles available)

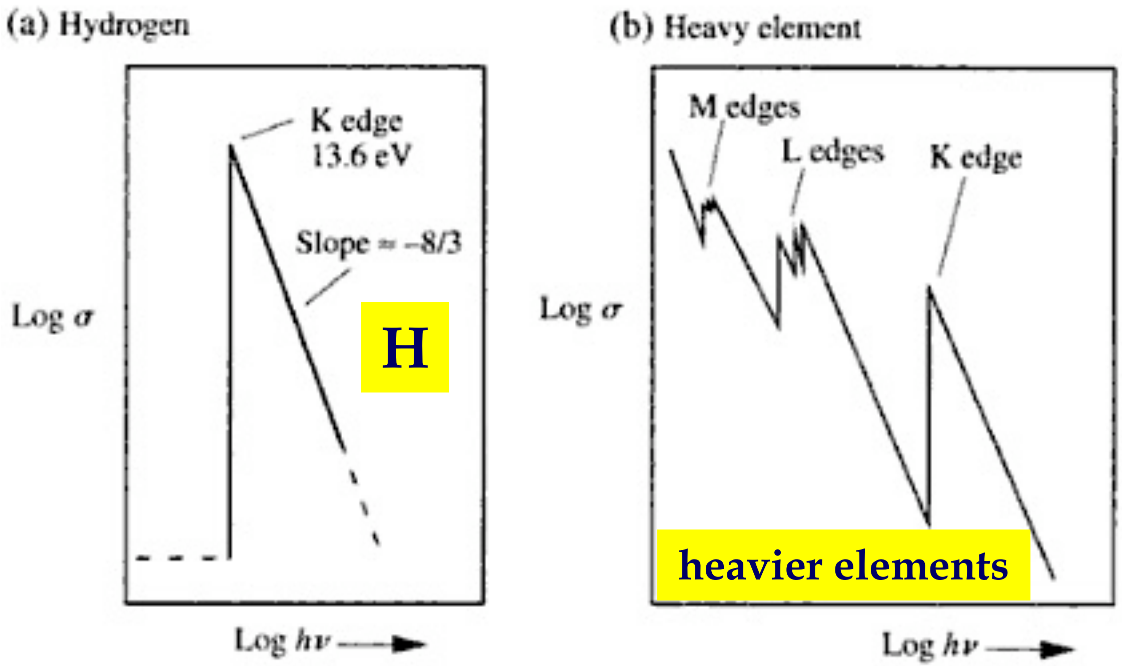
Photoelectric absorption



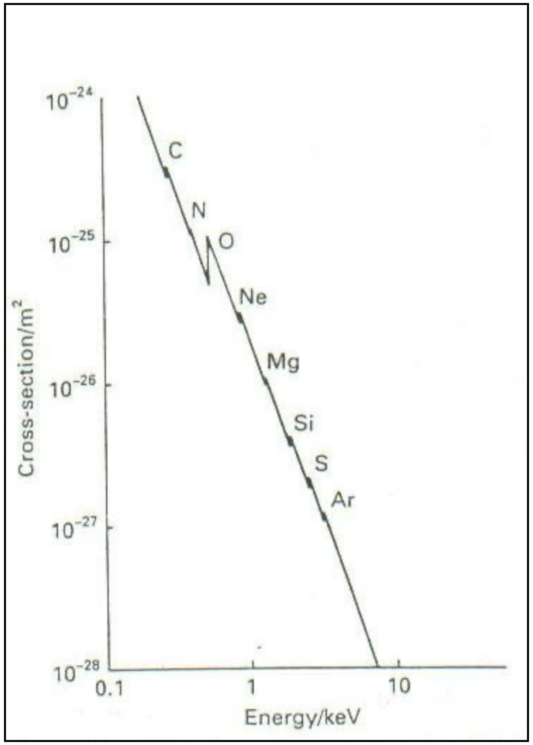
A bound electron is ejected from the atom by the absorption of a photon with $E \geq E_{th}$ with E_{th} being the ionization potential (13.6 eV for H). Above the threshold, the cross section is:

$$\sigma_{ph} = 4\sqrt{2}\sigma_T \alpha^4 Z^5 \left(\frac{mc^2}{E}\right)^{\frac{7}{2}}$$

Given the $E^{-3.5}$ dependence, the absorption is dominated by photons just above threshold.

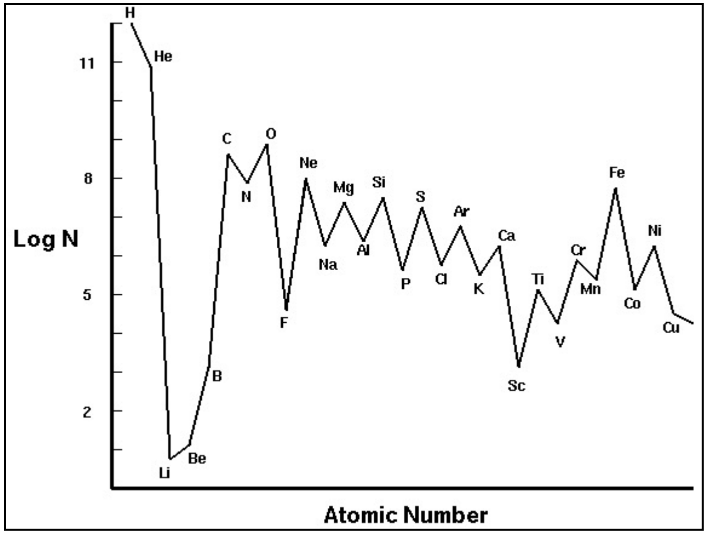


K shell requires higher energy photons

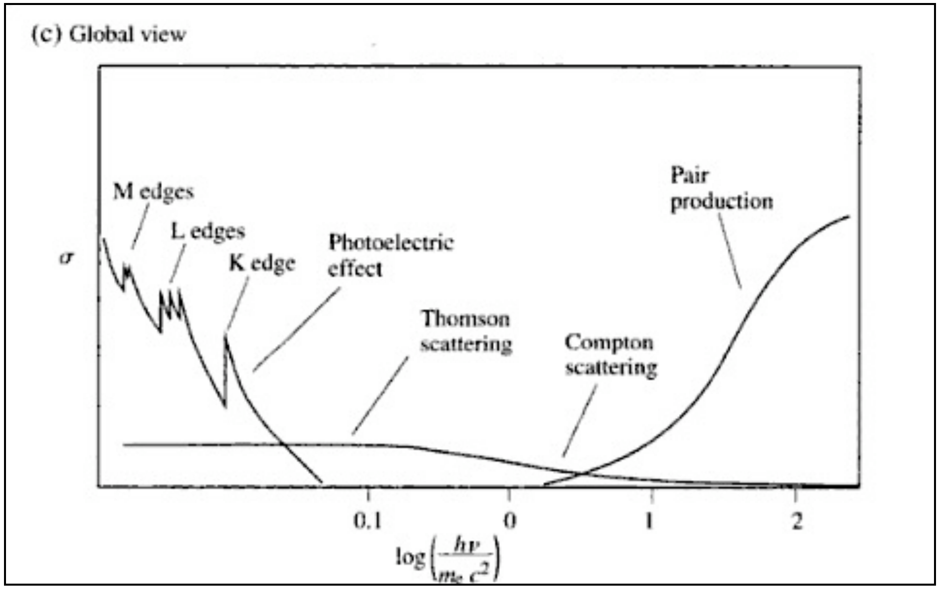


$$\sigma_{ph} = 4\sqrt{2}\sigma_T \alpha^4 Z^5 \left(\frac{mc^2}{E}\right)^{\frac{7}{2}}$$

Summing over all shells and convolving with cosmic element abundances, the total cross section can be derived

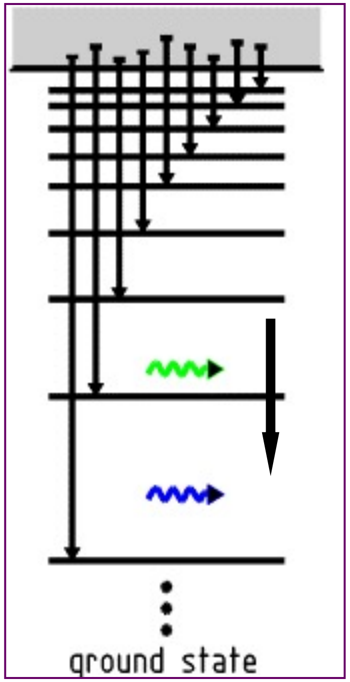


Photoionization is very important in the UV and soft X-ray band



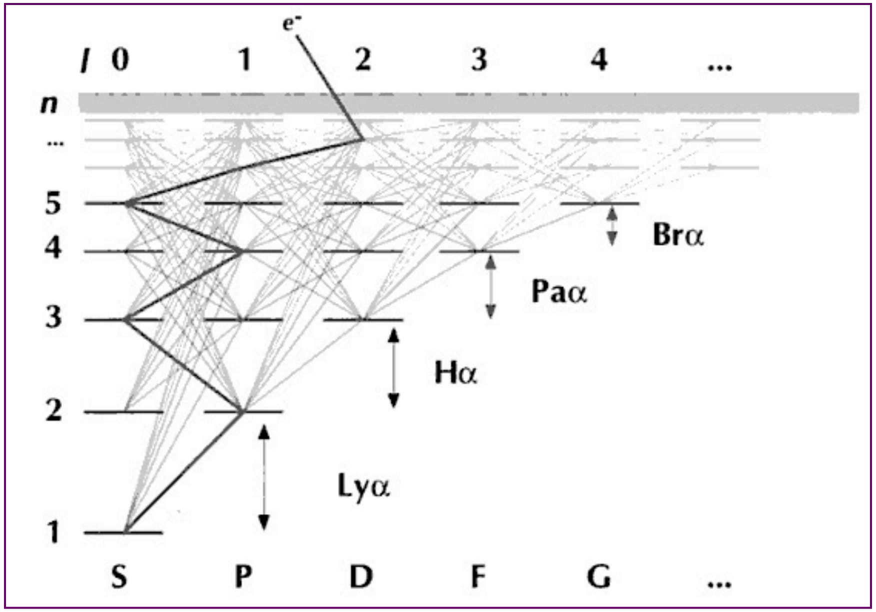
Radiative recombination

Radiative recombination (*free-bound*, i.e. the capture of an electron by an atom with release of one or more photons) can occur either via a recombination cascade (first the electron in an excited state with large principal quantum number) or directly to the ground state.



In the latter case, a pseudo-continuum is created, as the photon carries out the ionization potential plus the kinetic energy of the electron.

→ Radiative Recombination Continuum (RRC)



Emissivity of free-bound emission

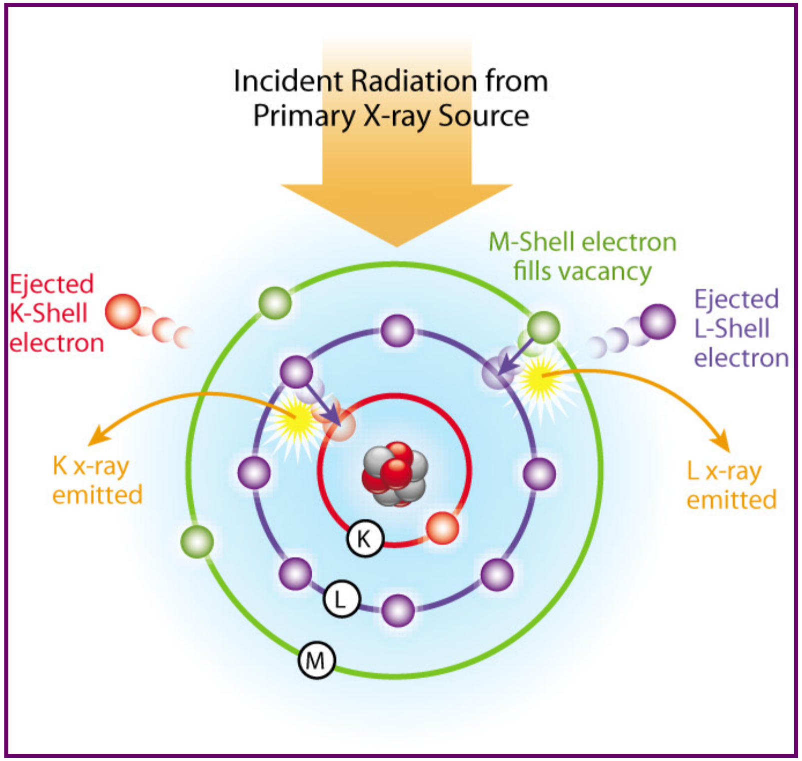
$$j_\upsilon = 5.44\times10^{-39}\left(\frac{Z^2}{T_e^{1/2}}\right)n_i n_e g_{fb}(\upsilon,Te)e^{-\frac{h\upsilon}{kT_e}}$$

g_{fb}=free-bound Gaunt factor

Recombination at work in e.g. PNe and HII regions (optical/near-IR)

- The emissivity is similar to that of the bremsstrahlung emission
- The recombination rate decreses with the electron velocity (temperature): at high temperature, electrons have higher speeds and are less likely to get captured

Fluorescence emission



If ionization occurs in an inner shell, the atom is not only **ionized** but also **excited**. De-excitation can occur via Auger effect (double ionization) or radiatively via emission of a *fluorescent photon*.

The probability of a radiative de-excitation is called *fluorescent yield*

$$Y \approx \frac{Z^4}{Z^4 + 33^4}$$

If the ionization is in the K shell, fluorescence may occur via a L→K (Kα photon), M→K (Kβ photon), etc.

Kα transition is the most probable (9/10 for iron)

The fluorescent yield of a shell represents the probability that a vacancy in that shell is filled by a radiative transition rather than by the ejection of Auger electrons.
For a sample of many atoms, this is equal to the number of photons emitted when vacancies in the shell are filled divided by the number of vacancies in the shell created by photoionization.

$$Y_Z^K \approx \frac{N_K}{n_{vK}}$$

N_K ← Number of K-shell X-ray photons emitted

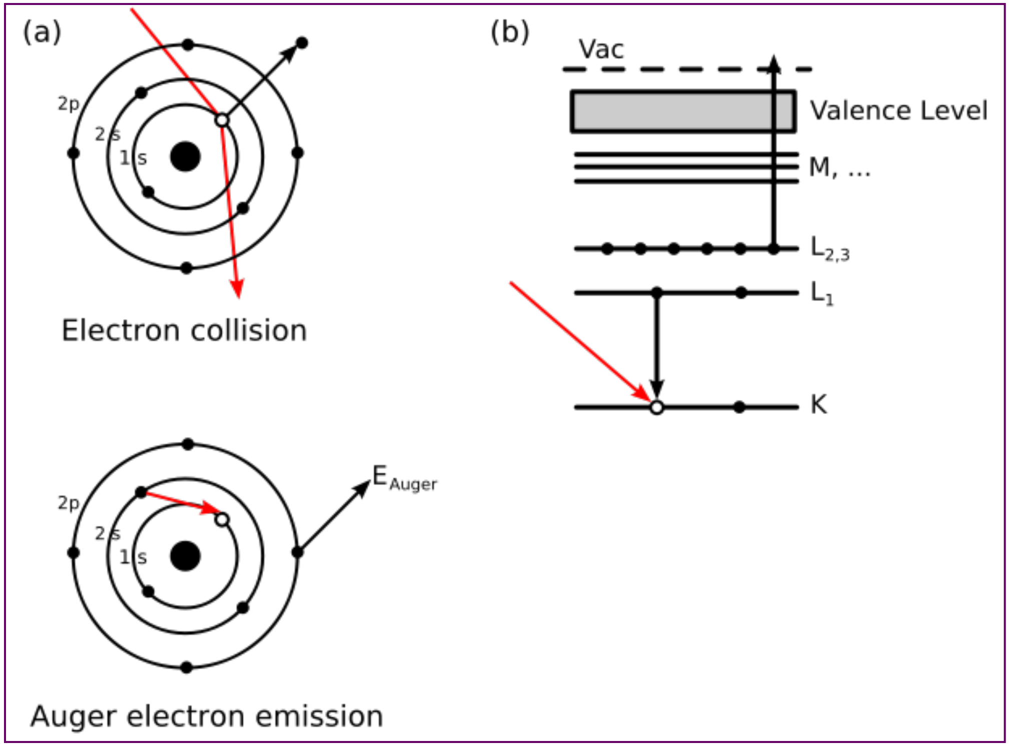
n_{vK} ← Number of primary vacancies

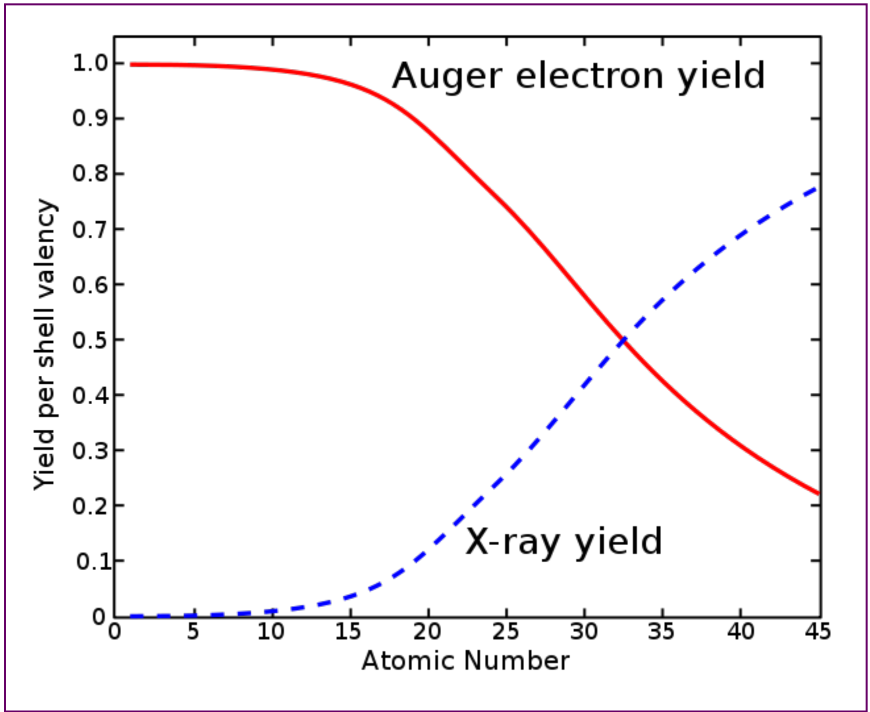
$Y_{Fe,K}$=0.34 (FeI) – 0.49 (FeXXII) – 0.75 (FeXXVI)

The intensity of the K-shell lines of a particular element in a plasma is proportional to the product of the fluorescent yield and the abundance of that element.
➔ Iron is the element with the highest product, thus it is widely observed in AGN

Auger effect (auto-ionization)

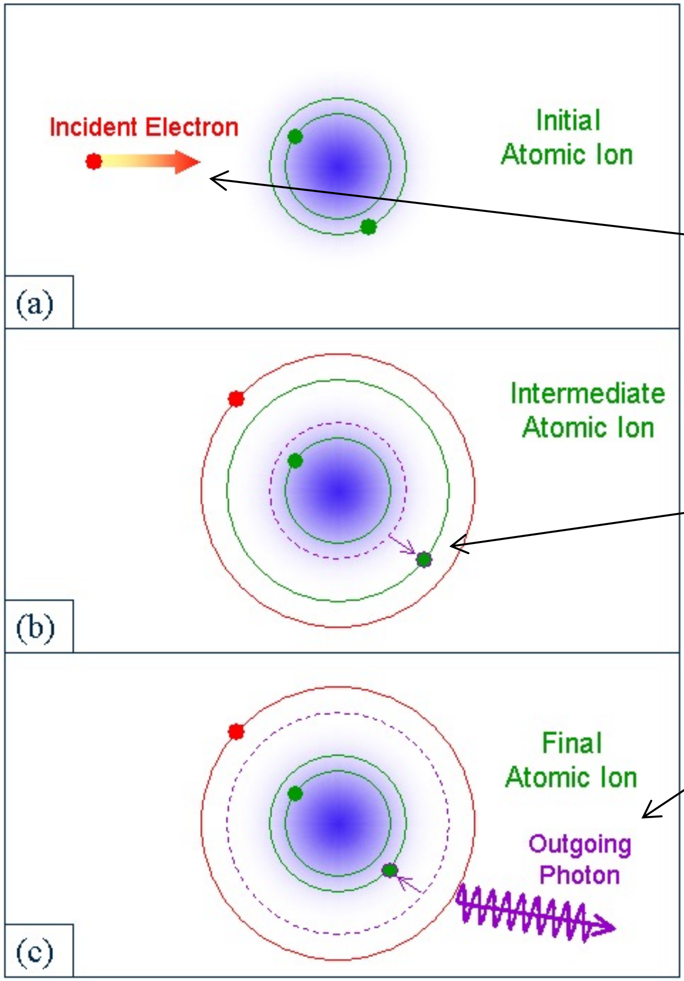
If a core-state (K-shell) electron is removed by a photon, thus leaving a hole, this can be filled by a outer-shell electron. The released energy (difference between the outer and the inner shells) kicks out another outer electron, which is called **Auger electron**.





Probability of occurrence of Auger vs. fluorescence

Dielectronic recombination



Dielectronic Recombination

an unbound electron finds itself bound to an atomic ion (an atom missing one or more of its electrons), with the "help" of one of the already bound electrons.

The excess energy is taken by a second electron which also occupied an excited state.

The doubly excited ion relaxes either by auto-ionizing or via radiative cascades.

This process is very important in determining the elemental abundances of cosmic gas clouds that are photo-ionized by energetic UV light.

Collisional equilibrium

Collisional Equilibrium (or coronal equilibrium): dynamical balance at a given temperature between collisional ionization from the ground states of the various atoms and ions in a plasma and the process of recombination from the higher ionization states.
Assumptions: matter in thermal equilibrium and negligible radiation field.
At equilibrium, ionization and recombination rates must be equal.

$$\left[C(X^{i},T)+\alpha(X^{i-1},T)\right]n(X^{i})n_{e}=C(X^{i-1},T)n(X^{i-1})n_{e}+\alpha(X^{i},T)n(X^{i+1})n_{e}$$

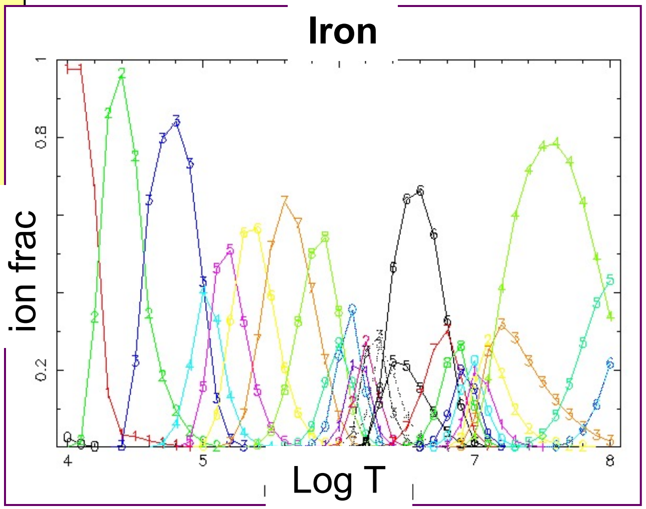
$n(X^{i})$ *density of i-th ion*

n_{e} *electron density*

$C(X^{i},T)$ *ionization coefficient of i-th ion (to i+1)*

$\alpha(X^{i},T)$ *recombination coefficient to i-th ion (from i+1)*

By solving this system of equations, the ionization equilibrium (i.e. the fraction of each ion of each element) can be obtained as a function of temperature



Line cooling

In collisionally ionized plasma, cooling by line emission may be important. Once solved for the ionization structure, and summing up the emissivity due to all ions, the total emissivity (integrated over frequencies) is: →

$$j_{lines} = \Lambda(T) n_i n_e$$
$$\Lambda(T) \propto T^{-0.7}$$

The main continuum emission process in a plasma is thermal bremsstrahlung →

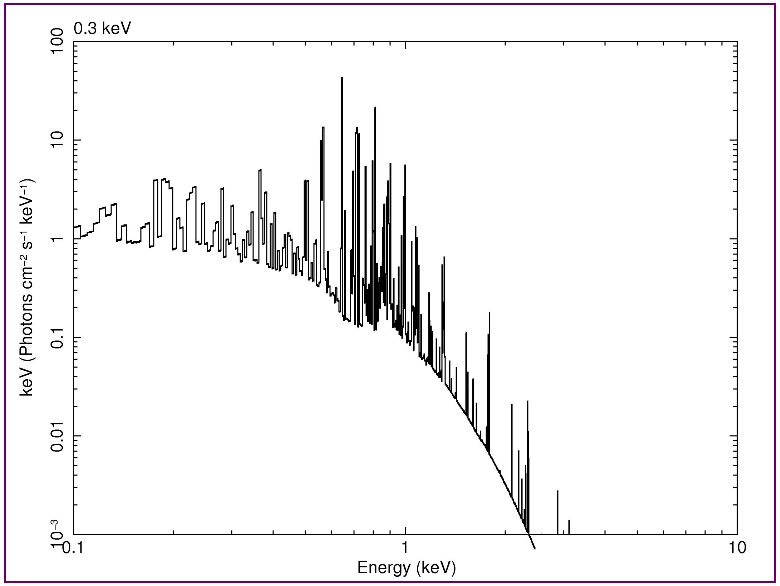
$$j_{br} \propto T^{\frac{1}{2}} n_i n_e$$

For cosmic solar abundances, bremsstrahlung dominates above ~2x10^7 K (i.e., about 2 keV), line cooling below

$$t_{\text{cool, br}} \propto (n_e + n_i)kT / j(T) \approx T^{1/2}$$
$$t_{\text{cool, lines}} \propto T / T^{-0.7} \approx T^{1.7}$$

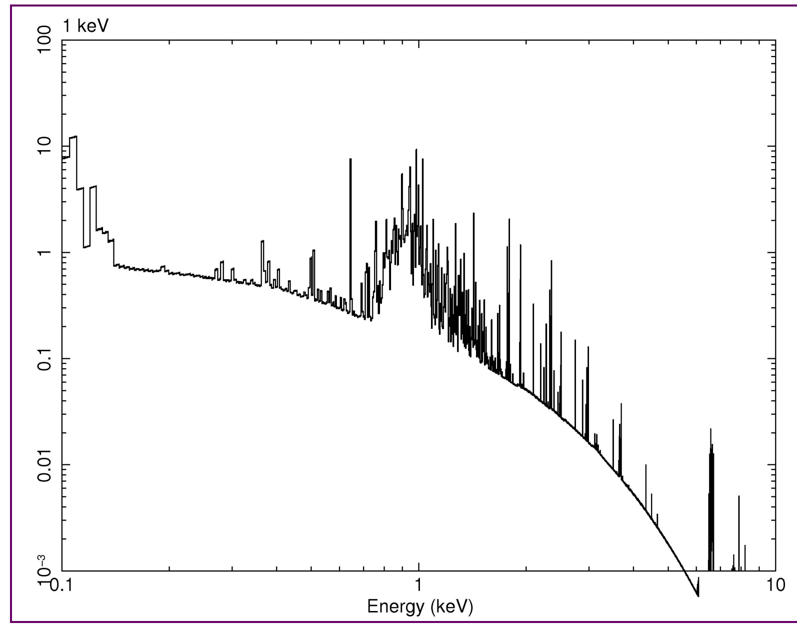
In the line-cooling regime, cooling becomes very fast

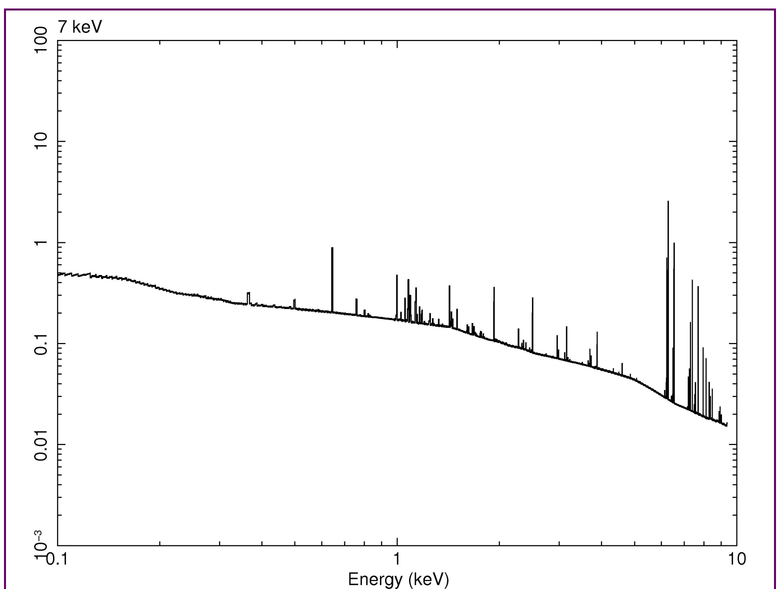
Spectra from collisionally ionized plasma



kT=0.3 keV – *line emission dominates*

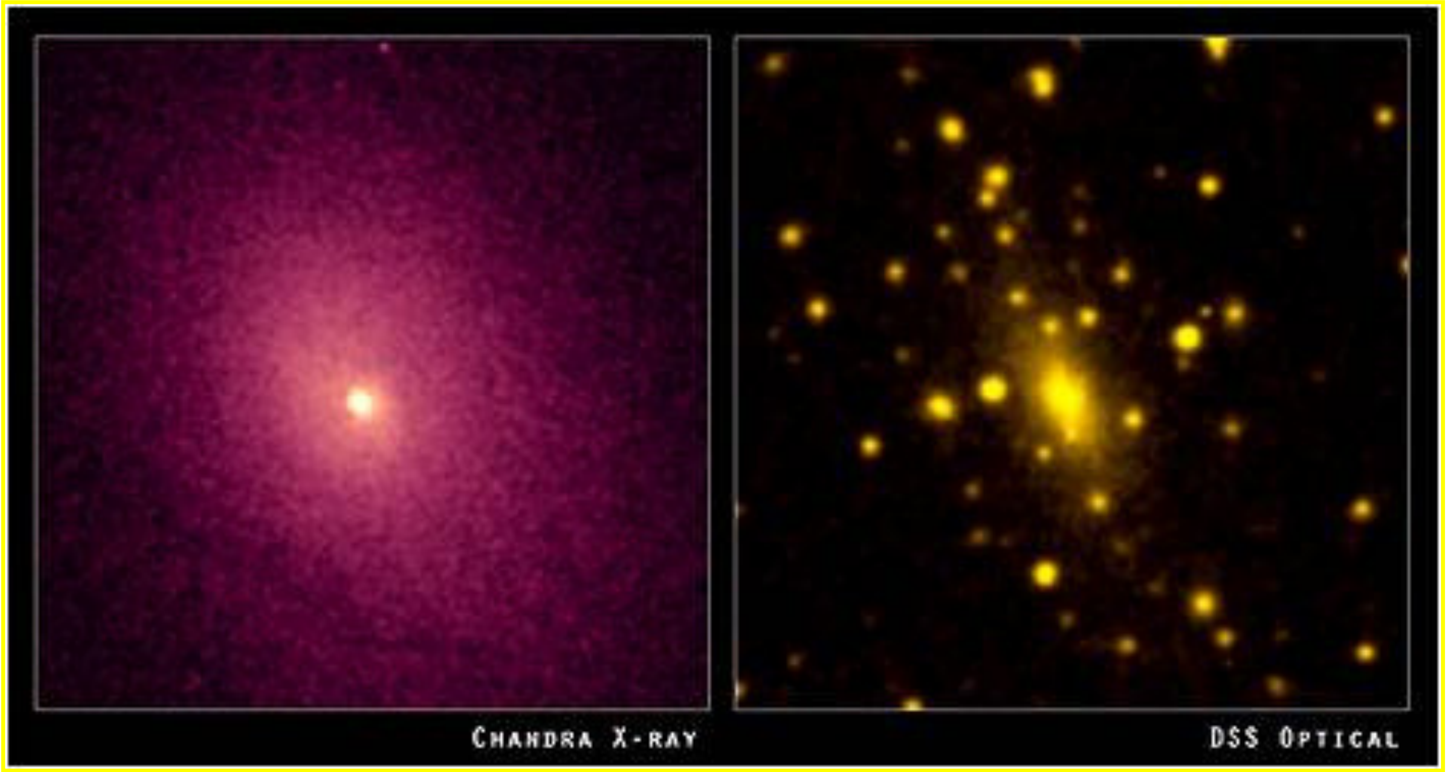
kT=1 keV – *line and continuum emission both important*





kT=7 keV – *continuum (brems.) emission dominates*

Example: Clusters of Galaxies



$$t_{eq}(e,e) \cong 3.3 \times 10^5 T_8^{\frac{3}{2}} n_{e,-3}^{-1}\ yrs$$

$$t_{eq}(p,p) \cong \sqrt{\frac{m_p}{m_e}}\, t_{eq}(e,e)$$

$$t_{eq}(e,p) \cong \frac{m_p}{m_e}\, t_{eq}(e,e) \approx 6 \times 10^8\ yrs$$

IGM (Inter Galactic Medium) is in collisional equilibrium

Photoionization equilibrium

Photoionization Equilibrium: matter is in equilibrium with the radiation field. Photoabsorption may now be the main ionization process.
At equilibrium, photoionization and recombination rates must be equal.

Assuming that the recombination time scale, $1/a(X^{i+1})n_e$, is short, we have:

$$n(X^i)\int_{\nu_0}^{\infty}\frac{F_\nu e^{-\tau_\nu}\sigma_\nu\left(X^i\right)}{h\nu}d\nu = \alpha(X^i,T)n(X^{i+1})n_e$$

$n(X^i)$ *density of i−th ion*

n_e *electron density*

σ_ν *photoelectric cross section*

$\alpha(X^i,T)$ *recombination coefficient*

The *ionization rate* depends on the ionizing photon flux, the *recombination rate* on the matter density.
The ionization structure is therefore governed by the so called *ionization parameter U*

U=ionization parameter=density of photons/density of electrons

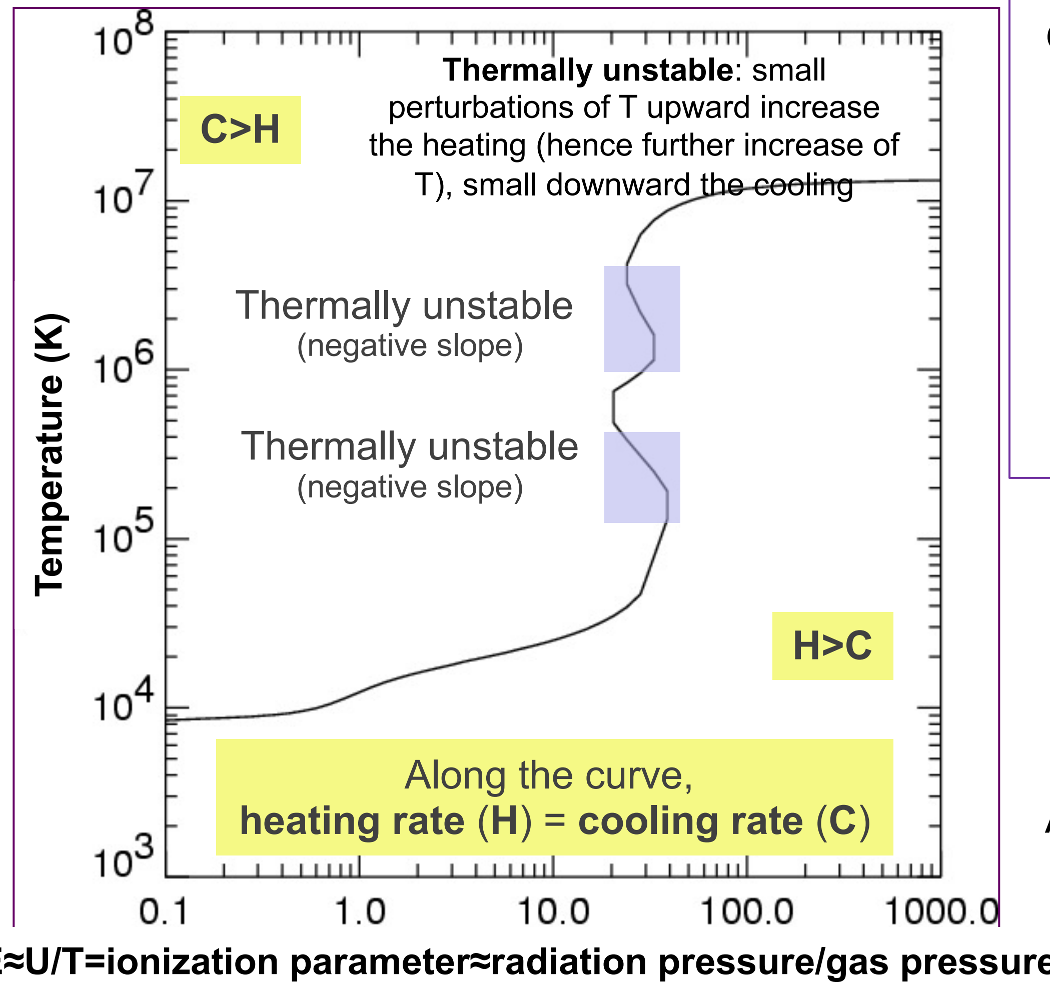
Number of photons

Ionization Parameters

$$U = \frac{\int_{\nu_0}^{\infty}\frac{F_\nu}{h\nu}d\nu}{n_e} \quad or \quad \Xi \propto \frac{U}{T} \propto \frac{\text{rad. pressure}}{\text{gas pressure}}$$

In the photoionization equilibrium, temperature does not change much with the ionization parameter until the matter is completely ionized.
At that point, photons can no longer be used for ionization, and the main interaction becomes Compton scattering

Curve of thermal stability



Isobaric perturbations have constant Ξ, and thus correspond to vertical displacements in the T vs. Ξ plane. In thermal equilibrium, if an isobaric increase in T leads to cooling dominating over heating, the equilibrium will be stable. If such increase in T leads to heating dominating over cooling, the equilibrium will be unstable

The *Compton temperature* is then reached

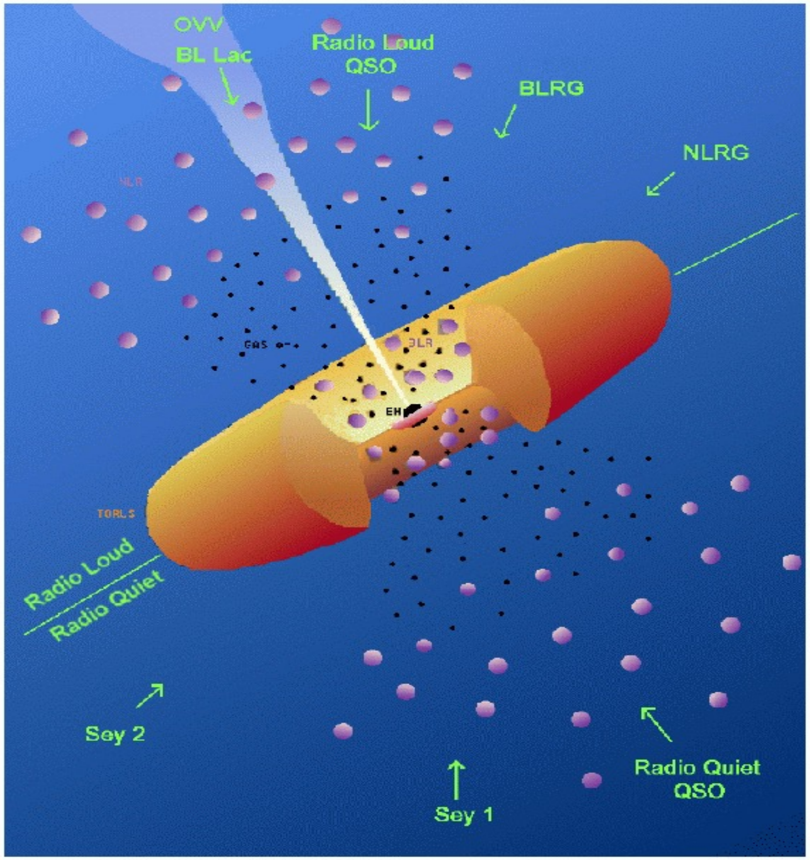
$$T_C = \frac{h\langle \nu \rangle}{4k}$$

At this temperature, the energy gained by the electrons is, on average, equal to the energy lost, so they are not further energized

Some AGN-related applications of emission processes (lines, continuum)

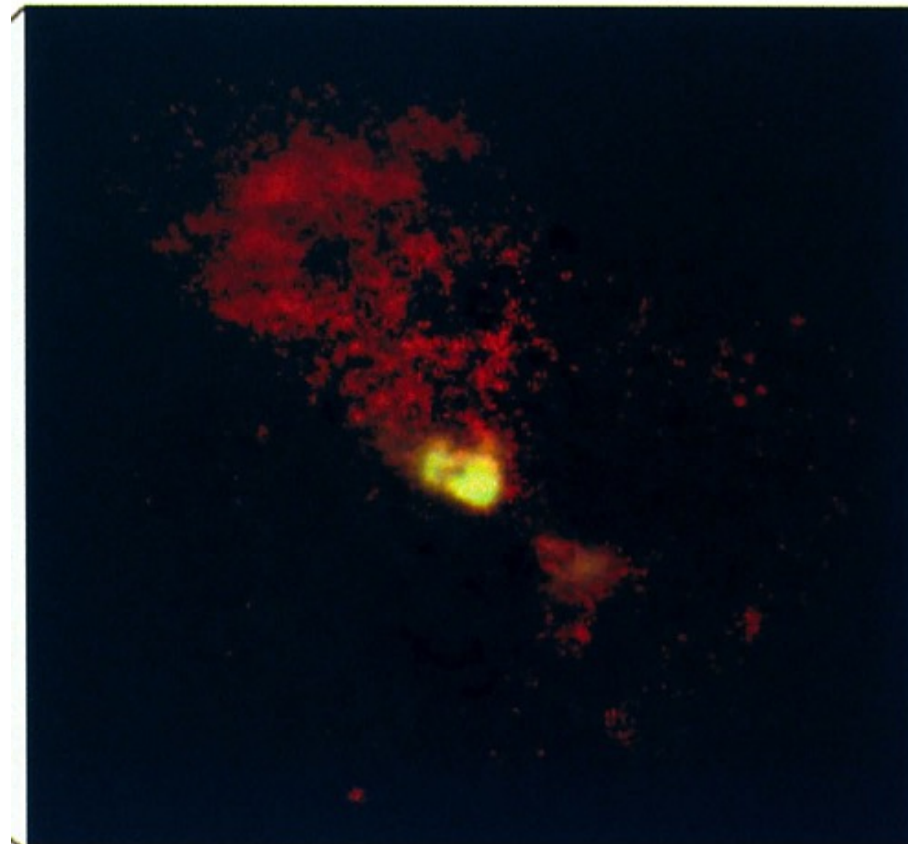
(to be expanded in further lessons of the course)

“Warm” reflectors in AGN



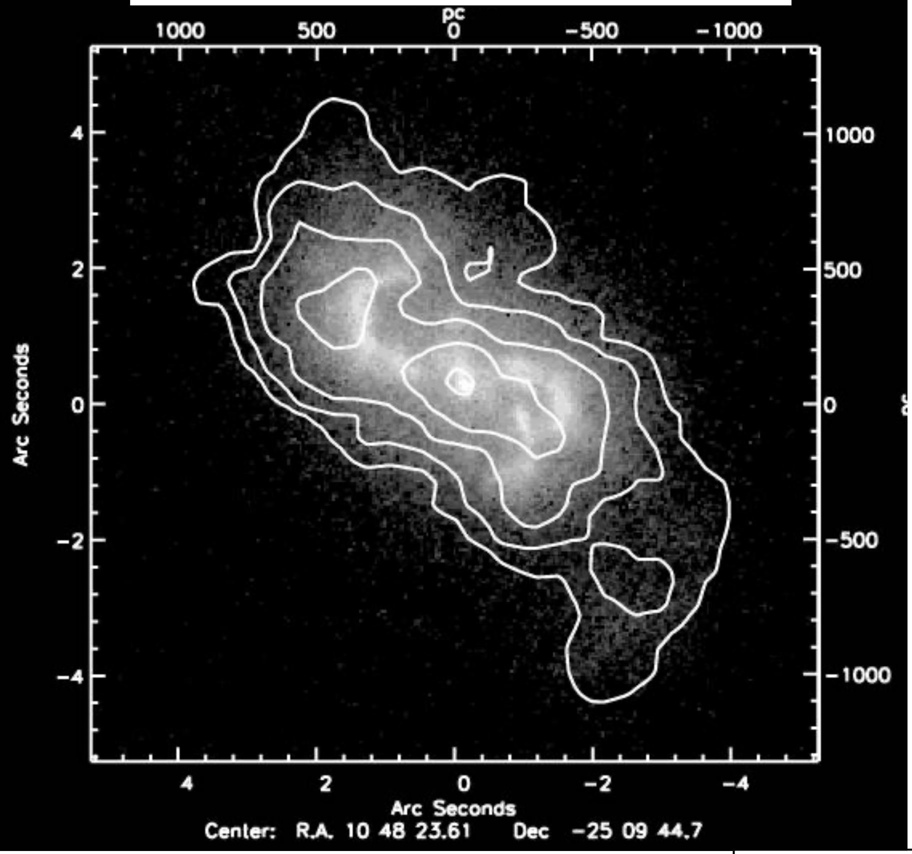
Urry & Padovani (1995)

NGC 5738 - HST

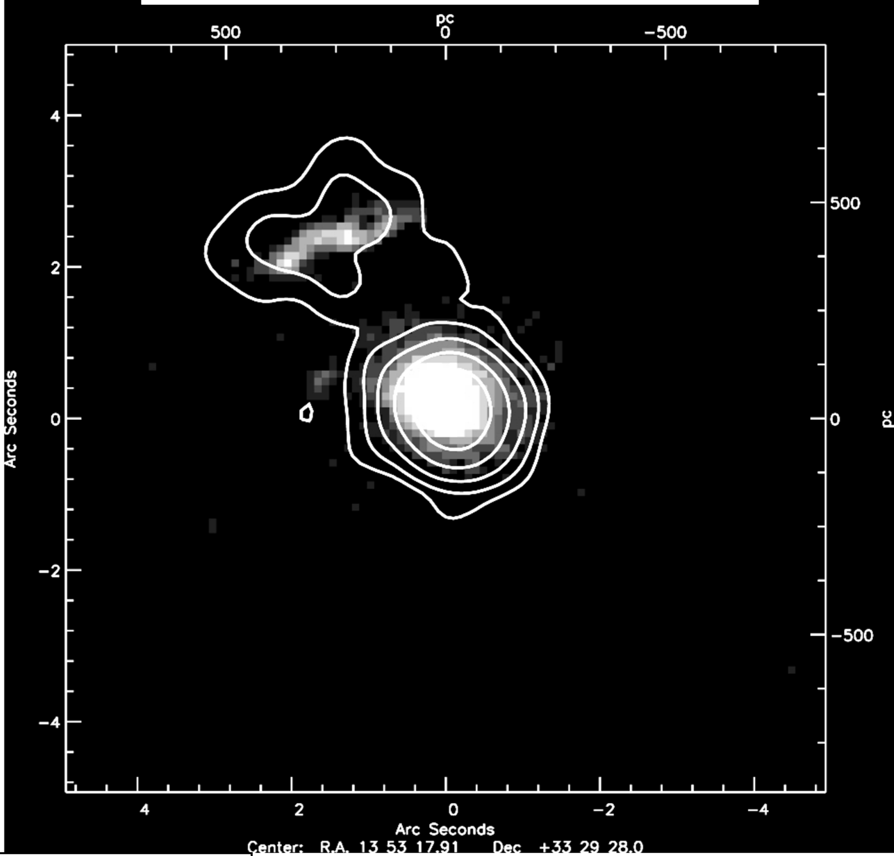


Spatial link between [OIII] (photoionization) and soft X-ray emission

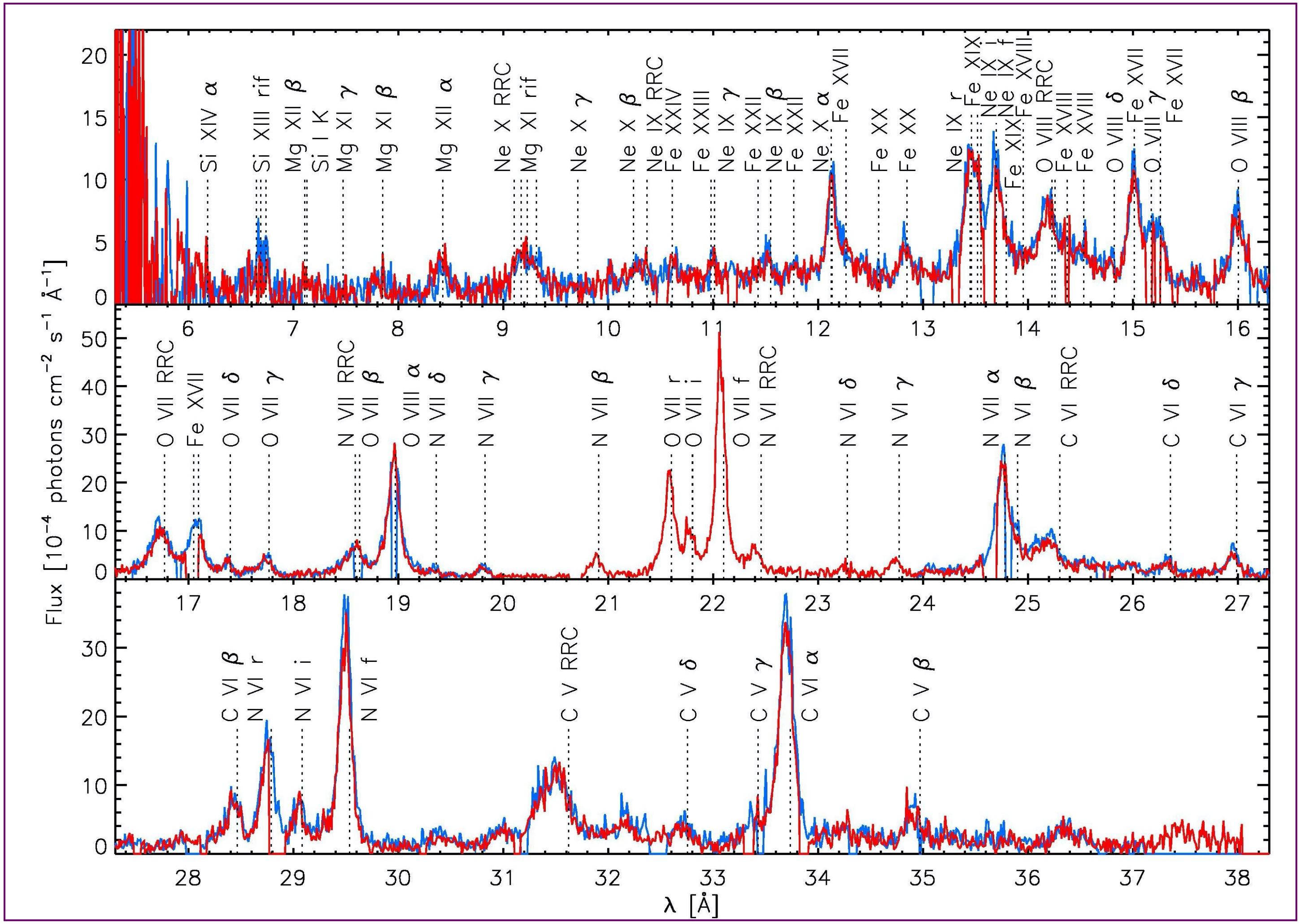
NGC 3393



NGC 5347



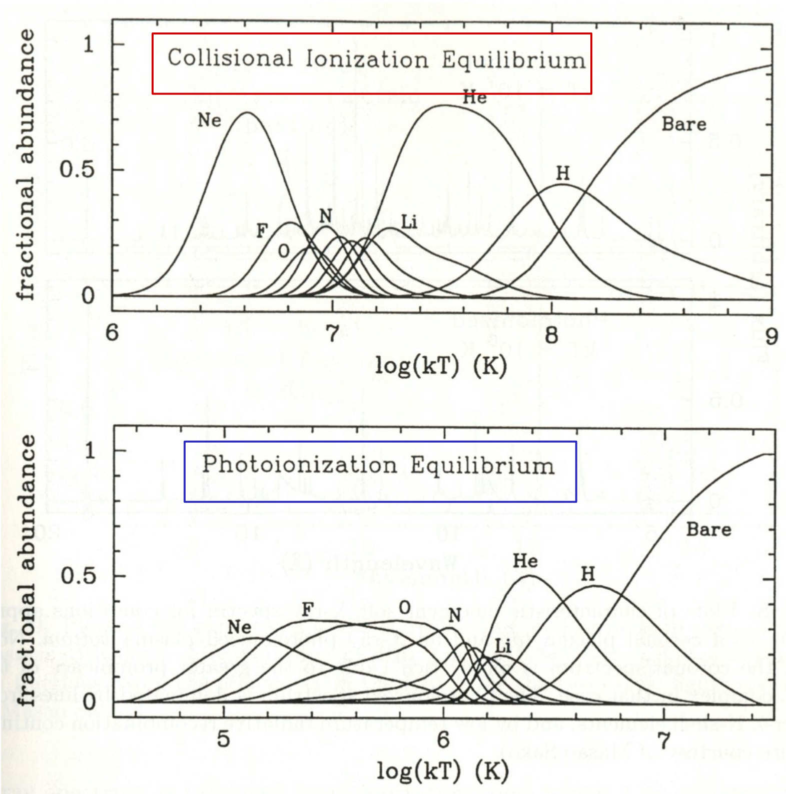
Bianchi et al. 2006

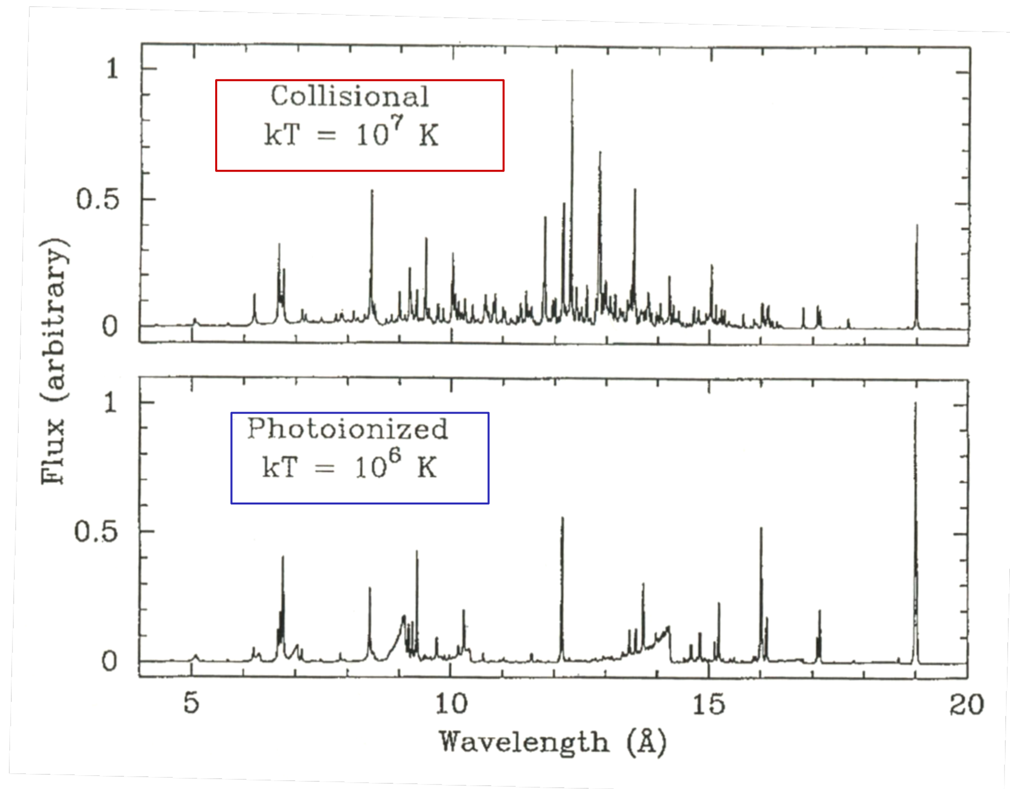


NGC 1068
(Kinkhabwala et al. 2002)

Is the soft X-ray emission spectrally consistent with photoionization?

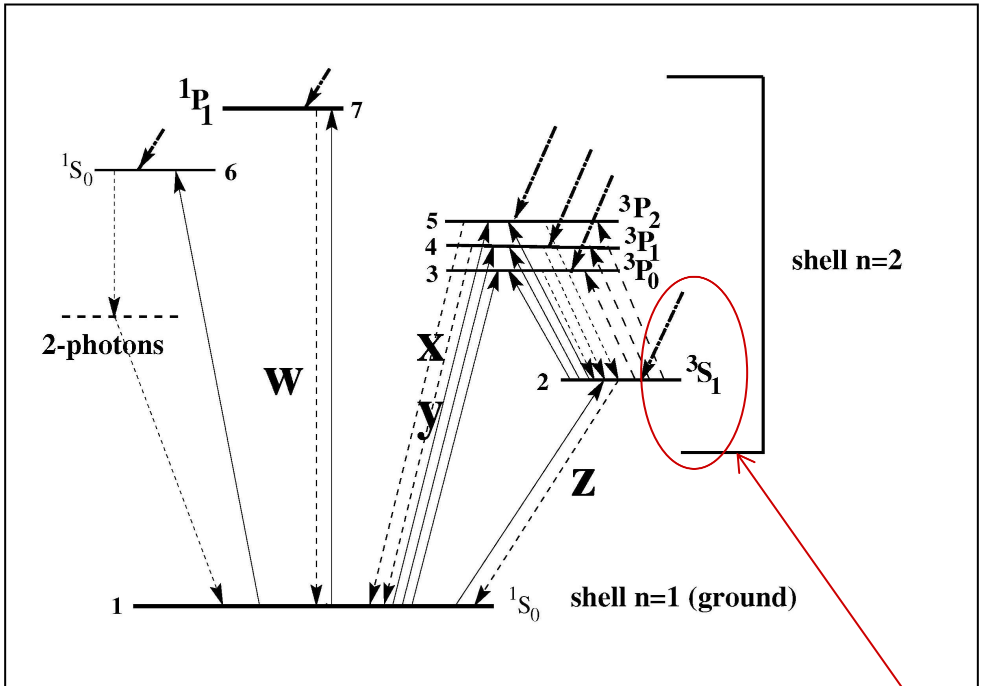
Collisional vs. photoionization spectra





Line diagnostics

Apart from the broad-band spectral fitting, other tools to distinguish between collisionally and photoionized plasma are:



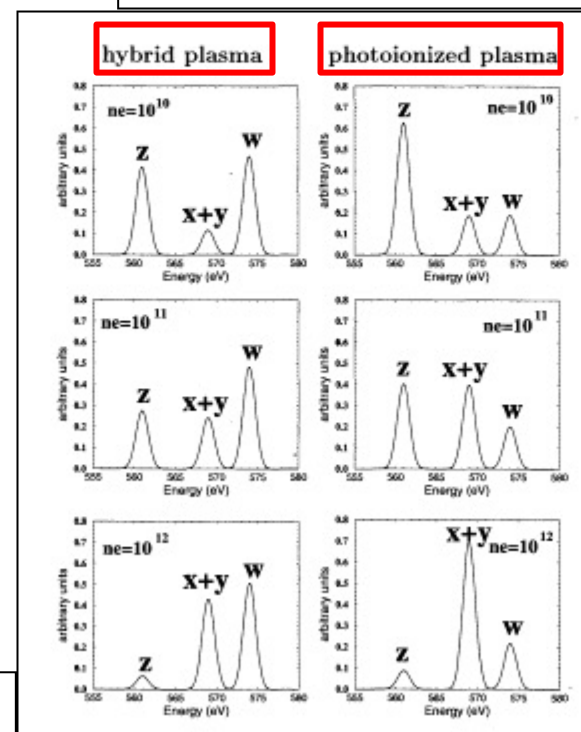
Radiative recombination preferentially occurs there

(*) A spectral line emitted in a transition between energy levels that have different values of the total spin quantum number (multiplicity)

Line ratios in He-like elements
(z=forbidden, w=resonant, x,y=intercombination(*))
Also density diagnostic

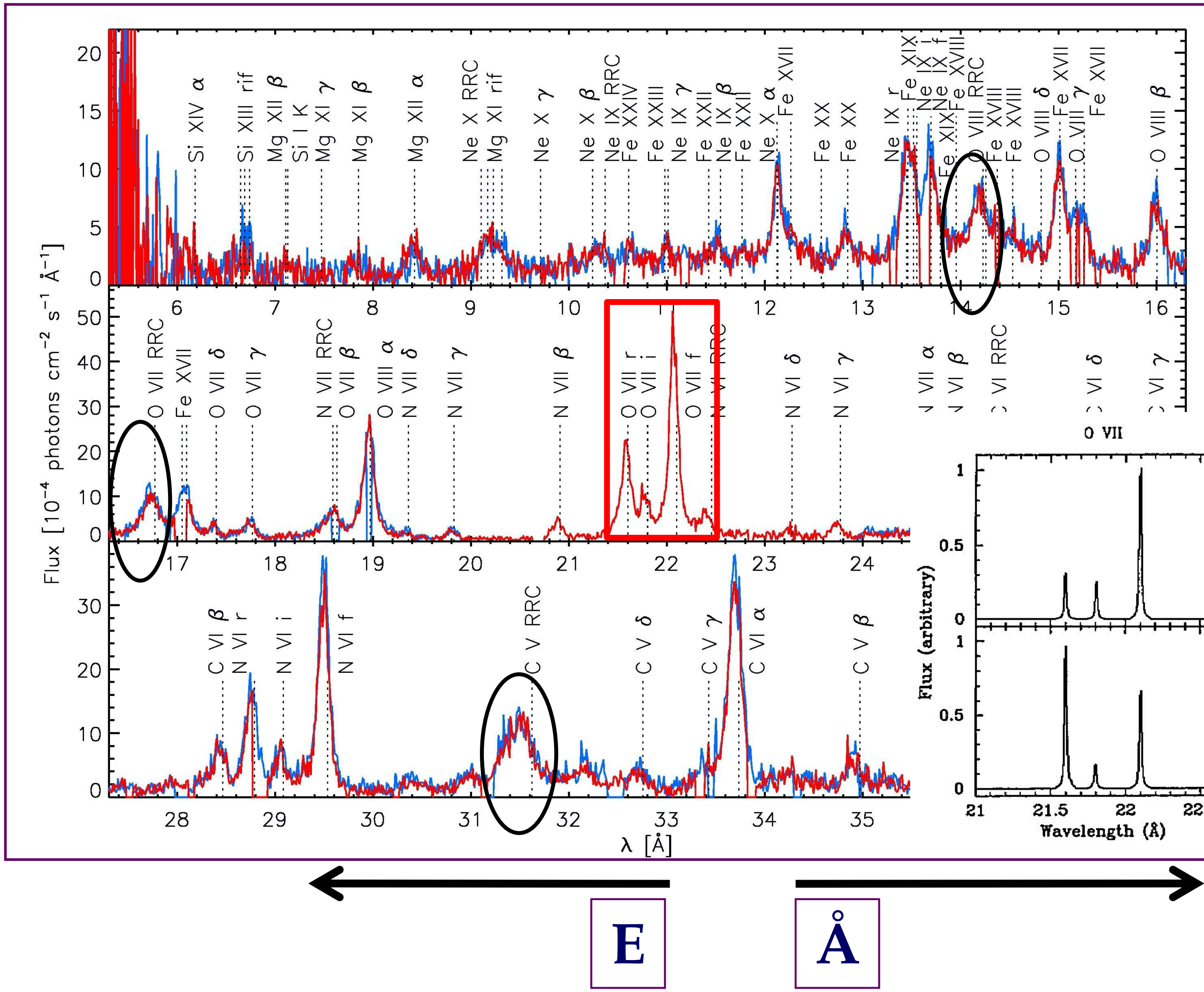
OVII line (soft X-rays)

n_e

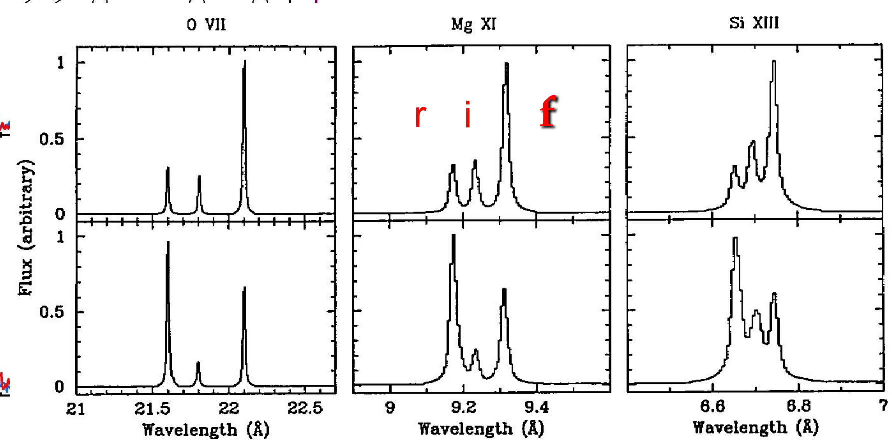


Porquet & Dubau 2000

The presence of prominent radiative recombination continua (RRC) features also indicates photoionized plasma (in collisionally ionized plasma it would be very broad and hard to detect)

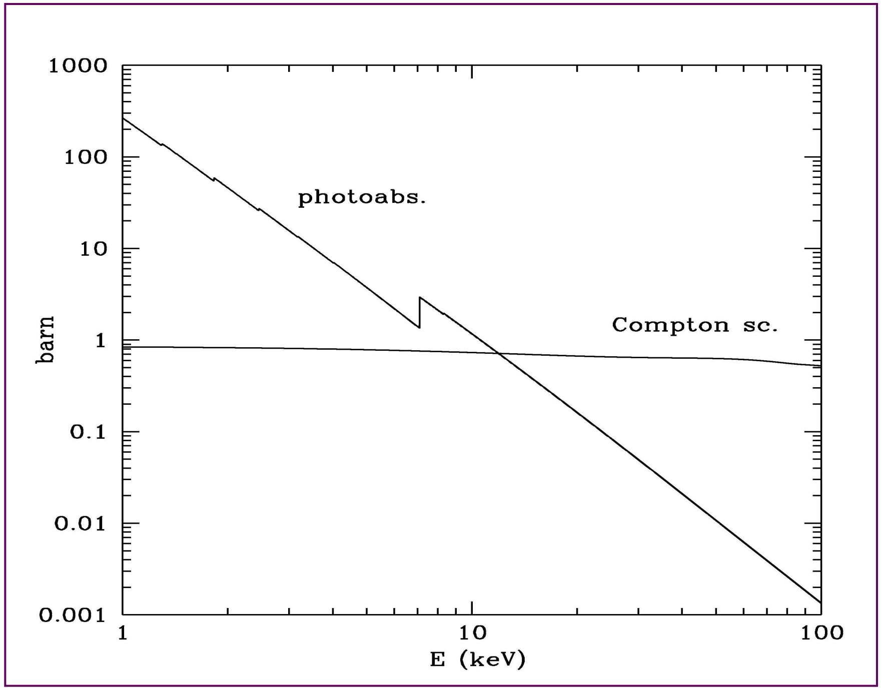


Top: photoionization
Strong forbidden line



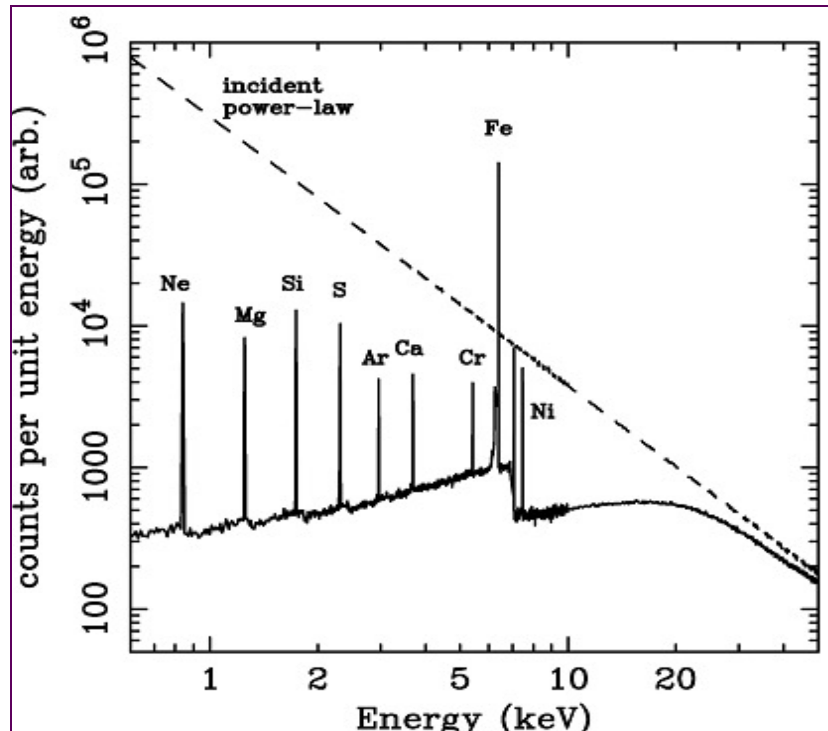
He-like atoms

Compton reflection

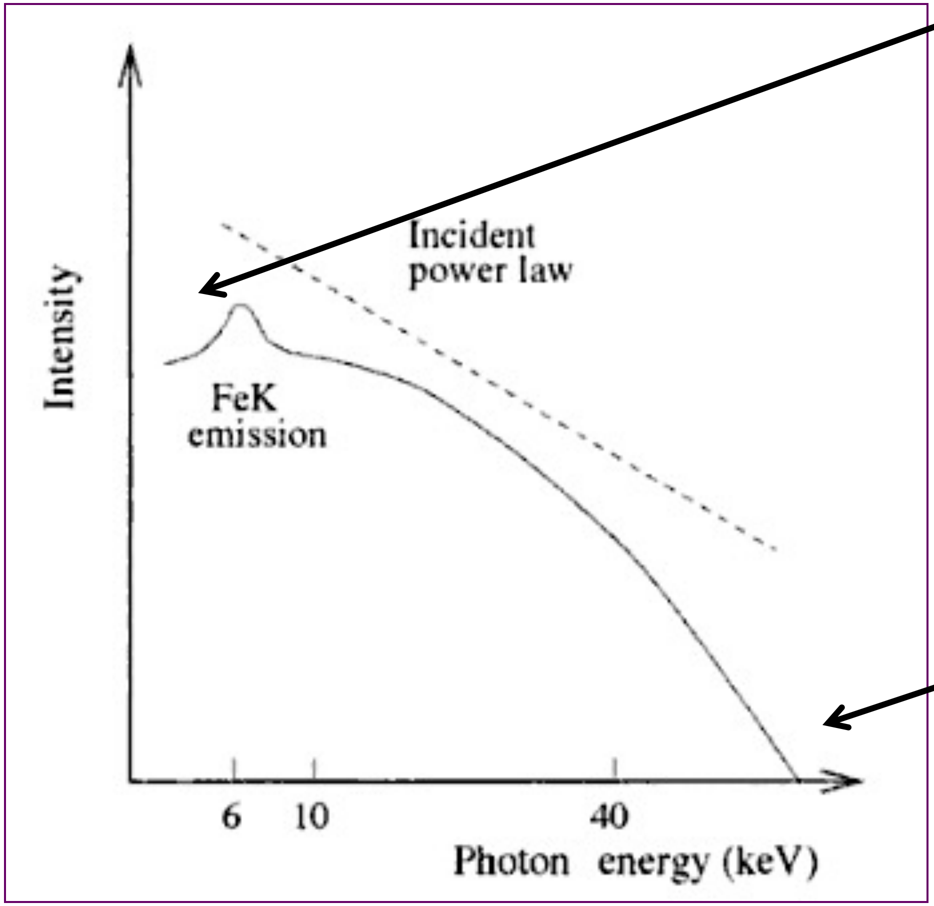


A rather common astrophysical situation is when X-rays illuminates `cold' matter. It produces the so called *Compton reflection continuum*

The shape of the continuum is due to the competition between photo-absorption and Compton scattering. Fluorescent lines are also produced, Fe Kα being the most prominent.



(Reynolds et al. 1995)

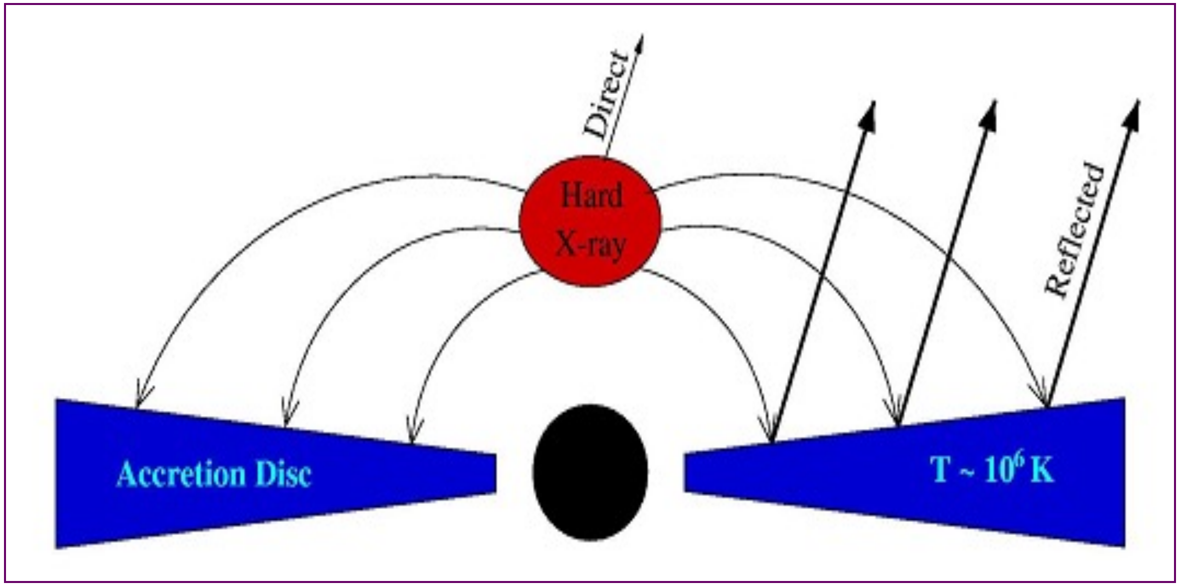


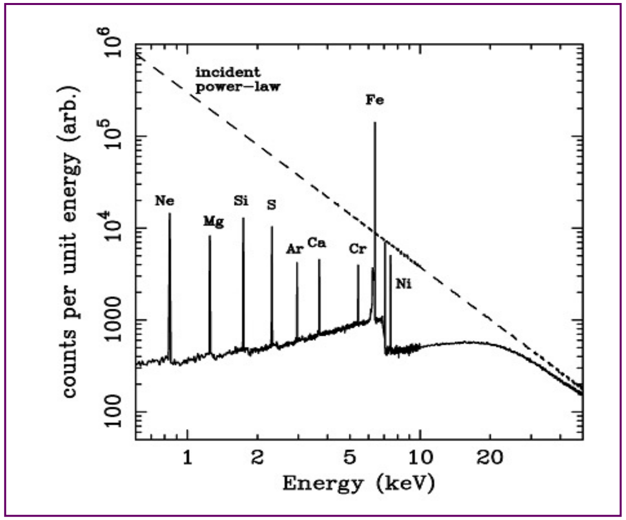
Attenuation due to photoelectric absorption

Energy loss due to Compton recoil

Iron line spectroscopy as General Relativity probe

Iron line can be used to probe General Relativity effects around Black Holes in Active Galactic Nuclei and Galactic Black Hole systems

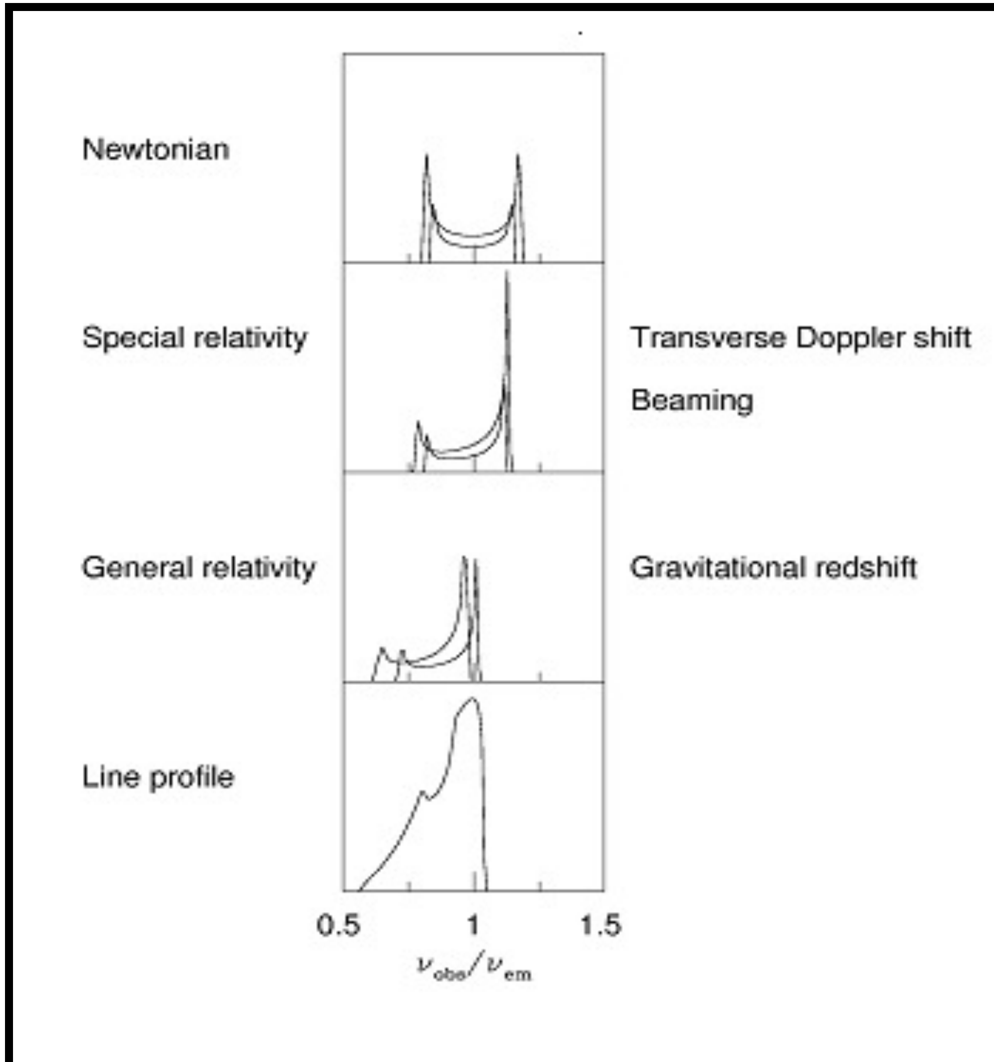




Iron line profiles

Line profile modified by SR and GR effects

Extended discussion in X-ray binaries and AGN lessons



(Fabian et al. 2000)