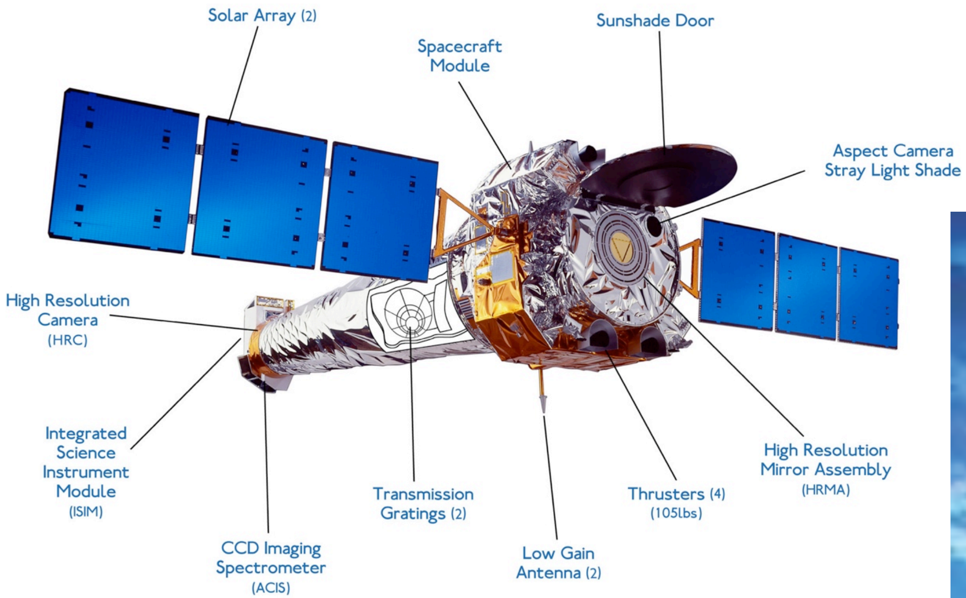
Atomic Physics for X-ray Astronomy at high spectral resolution

Julia C. Lee
Harvard University

with thanks to Frits Paerels, Randall Smith
for some slides and verbiage!

The Golden Age of X-ray Satellites



XMM-Newton

Chandra

X-ray band: ~ 0.1 - 100 keV

Extant: Suzaku, RXTE - 2009?, (BeppoSAX - 2003),
Planned: Astro-H, IXO
(Gamma Ray: Swift, Integral)

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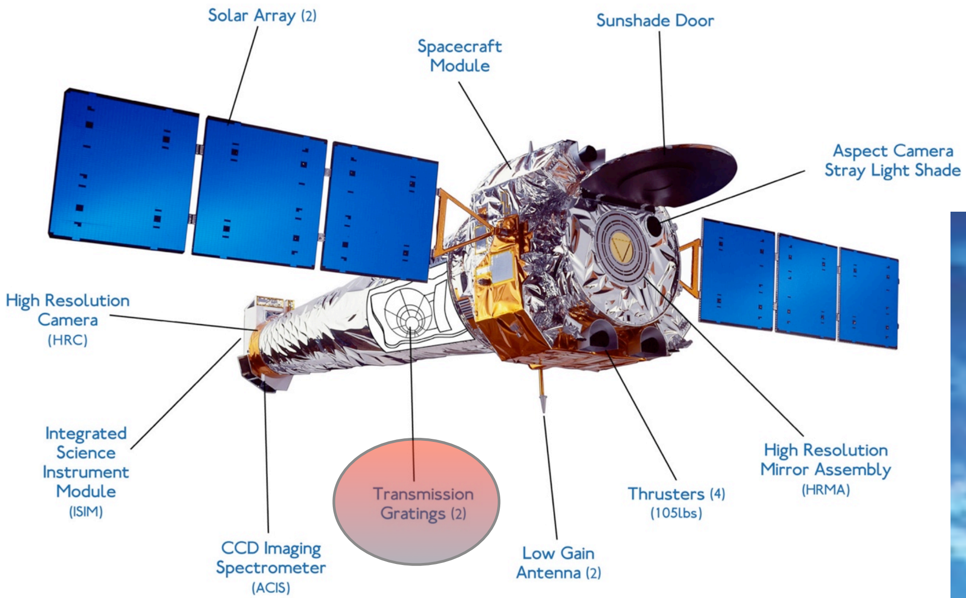
The Golden Age of X-ray Satellites



Chandra

XMM-Newton

In addition to on-board CCD Spectrometers:

- Chandra H(L)ETGS: High (Low) Energy Grating Spectrometers
- XMM-Newton RGS: Reflection Grating Spectrometer

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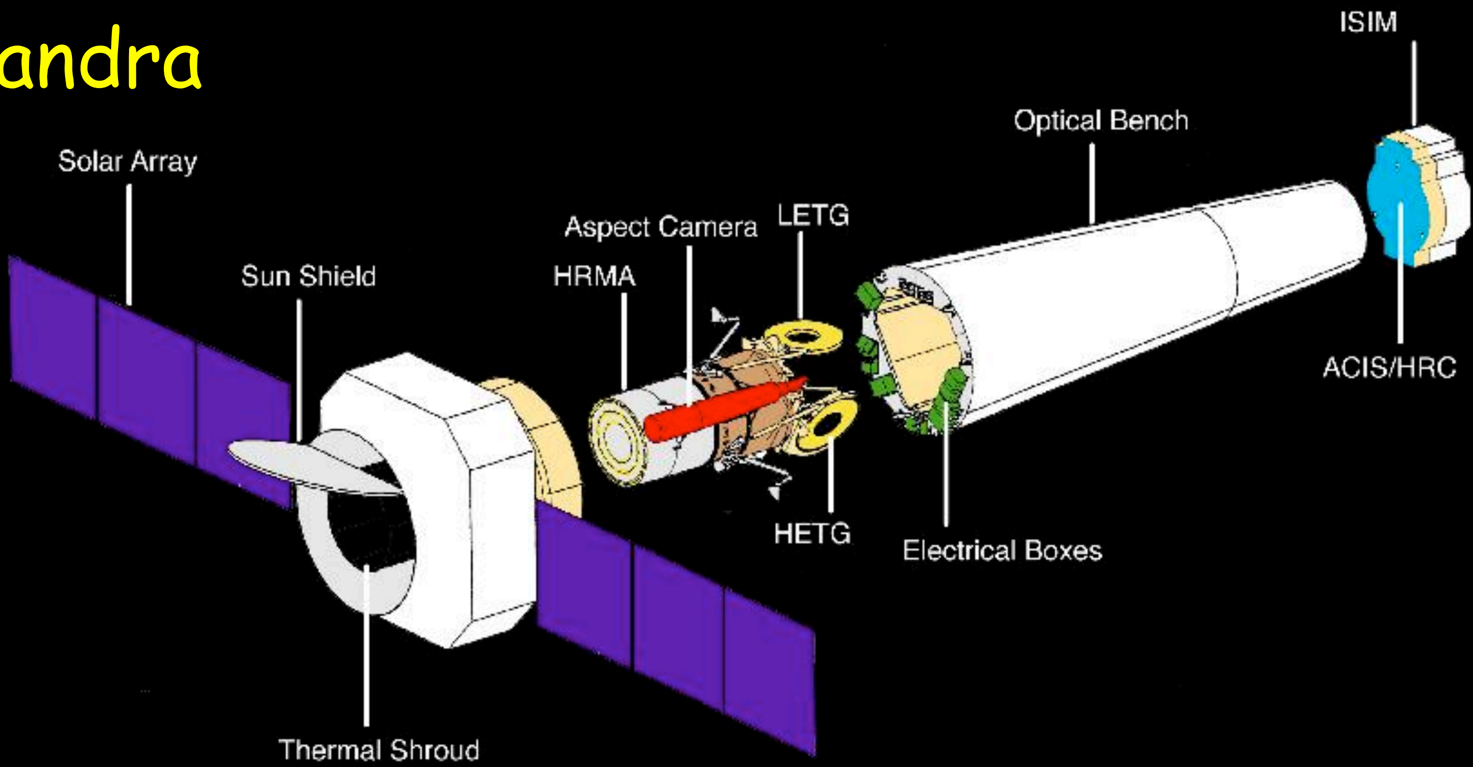
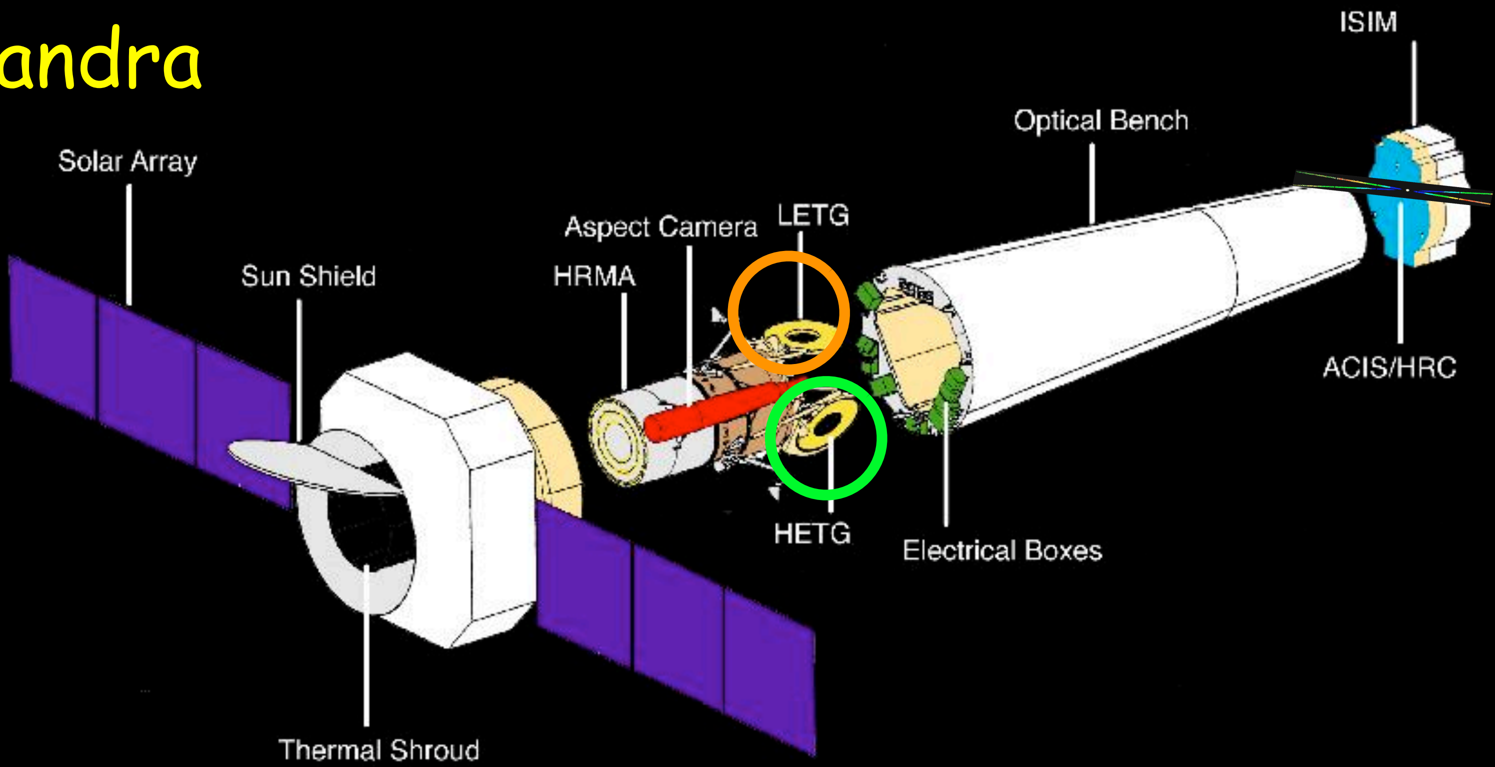
Chandra



ISIM
Optical Bench
Solar Array
Aspect Camera
LETG
Sun Shield
HRMA
ACIS/HRC
HETG
Electrical Boxes
Thermal Shroud

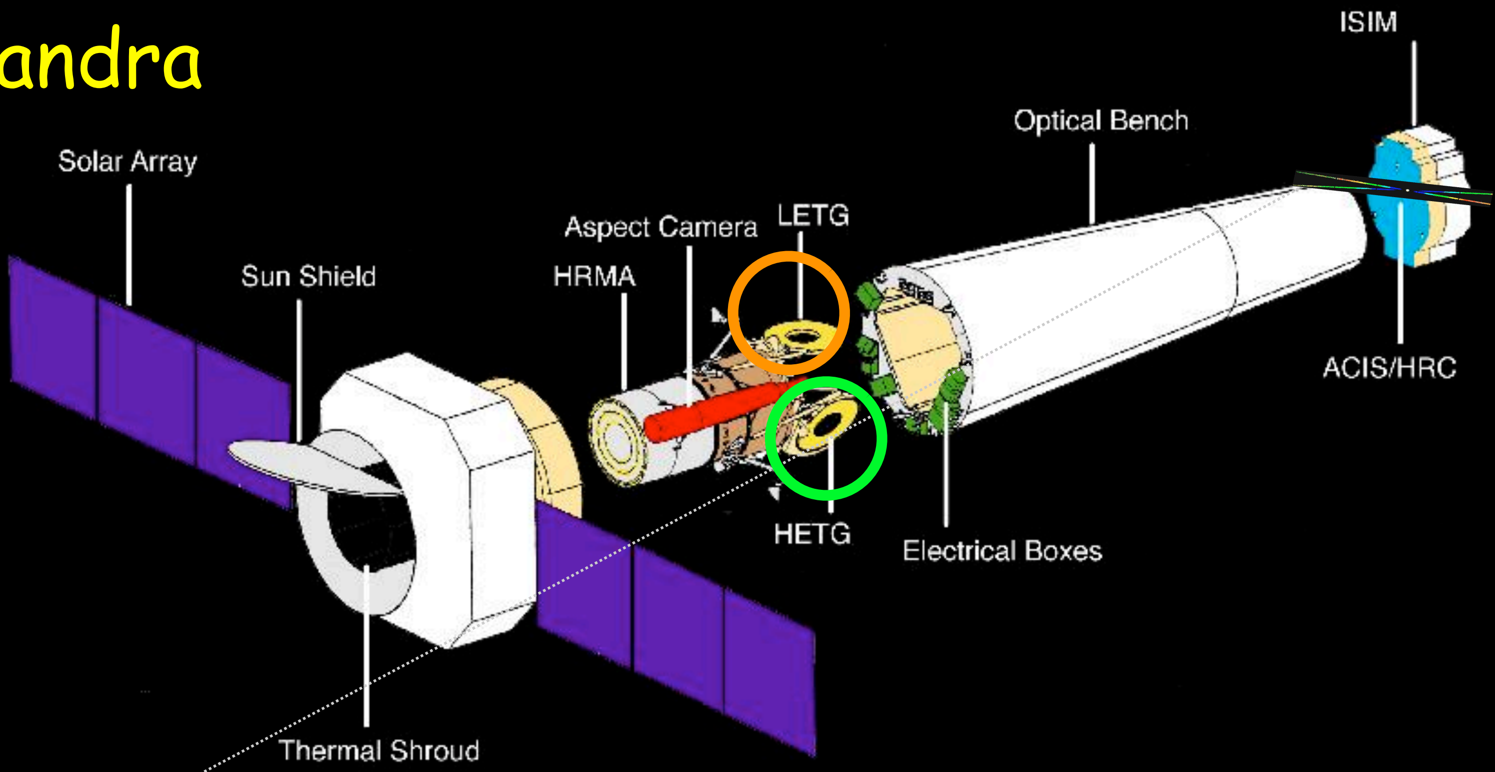
Chandra



HETGS: PI: Canizares (MIT)

LETGS: PI: Brinkmann? (Netherlands)

Chandra



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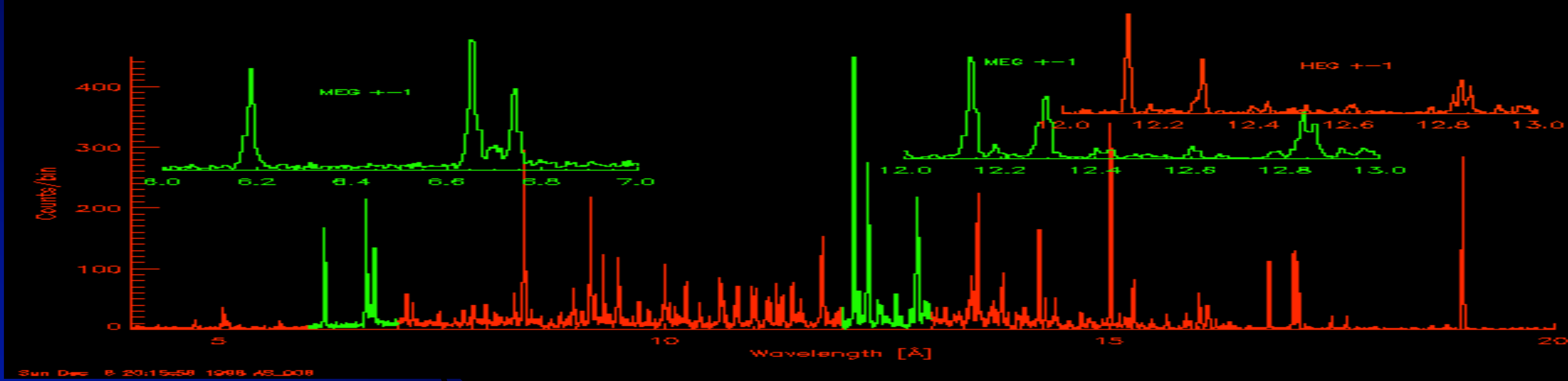


Spectral Resolution is key

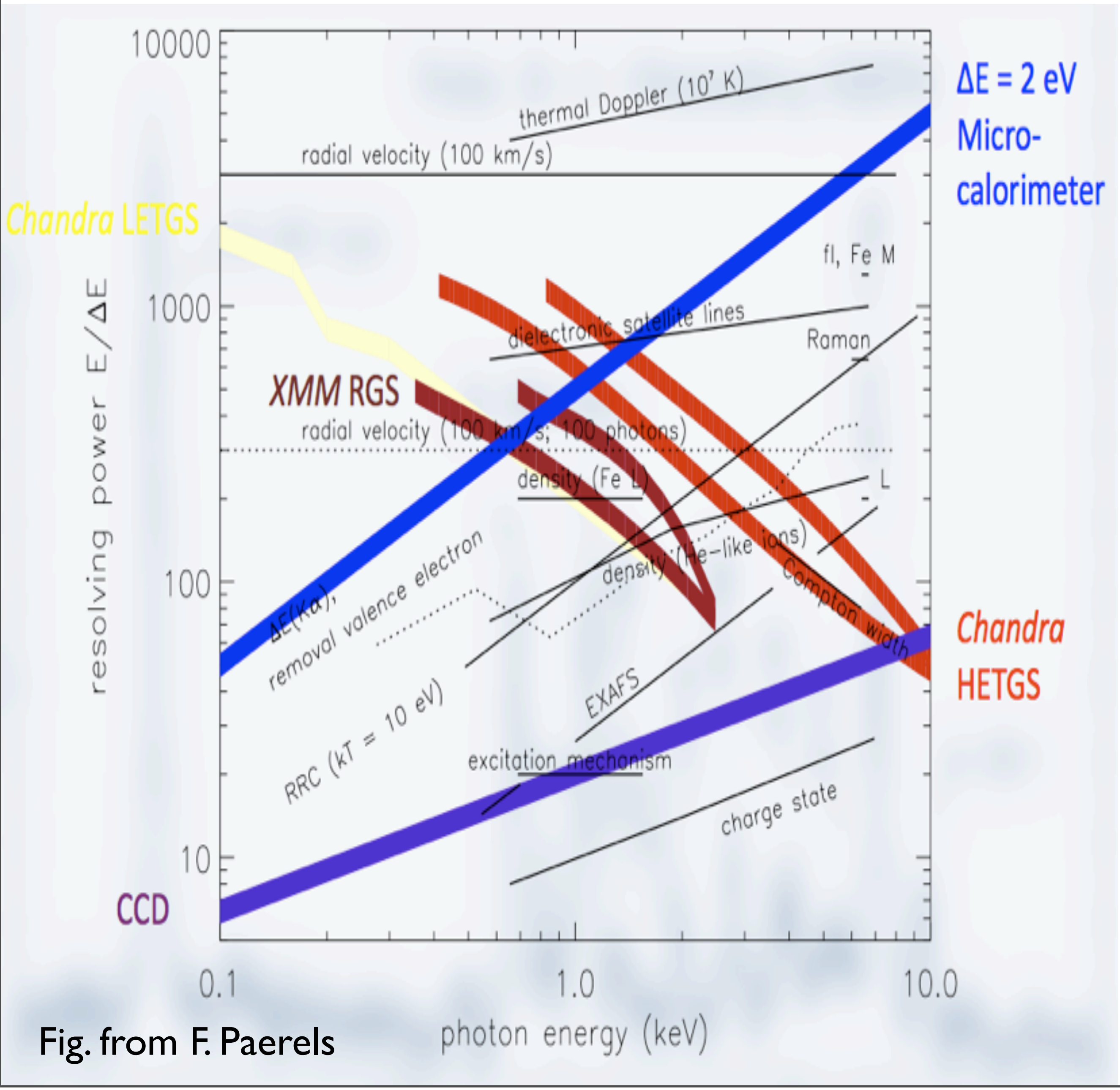


Fig. from F. Paerels

FWHM resolution

Chandra :

$\Delta\lambda_{HEG}$ = 0.012 A

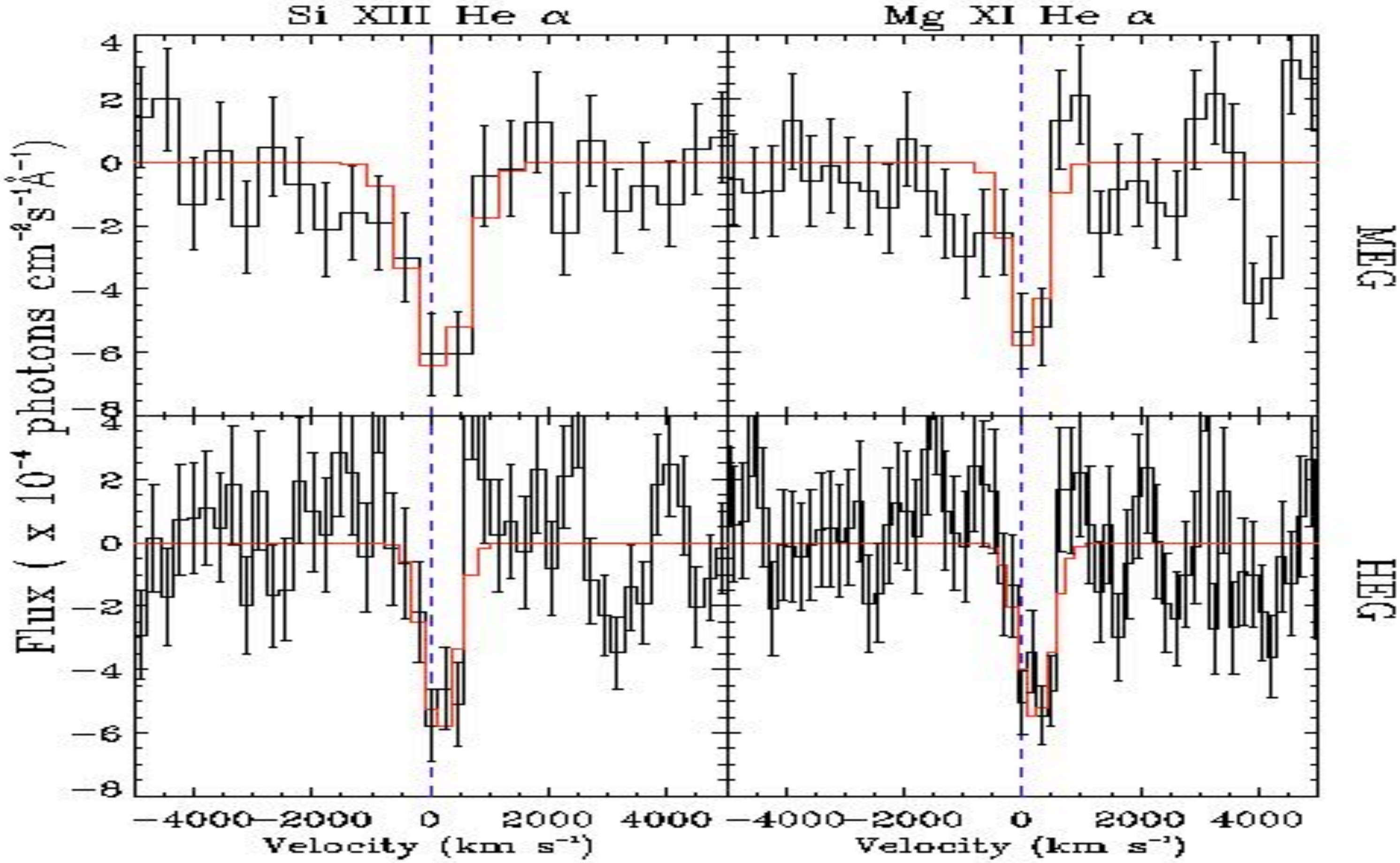
$\Delta\lambda_{MEG}$ = 0.023 A

$\Delta\lambda_{LETG}$ = 0.05 A

XMM-Newton :

$\Delta\lambda_{RGS}$ = 0.06 A

MEG vs. HEG



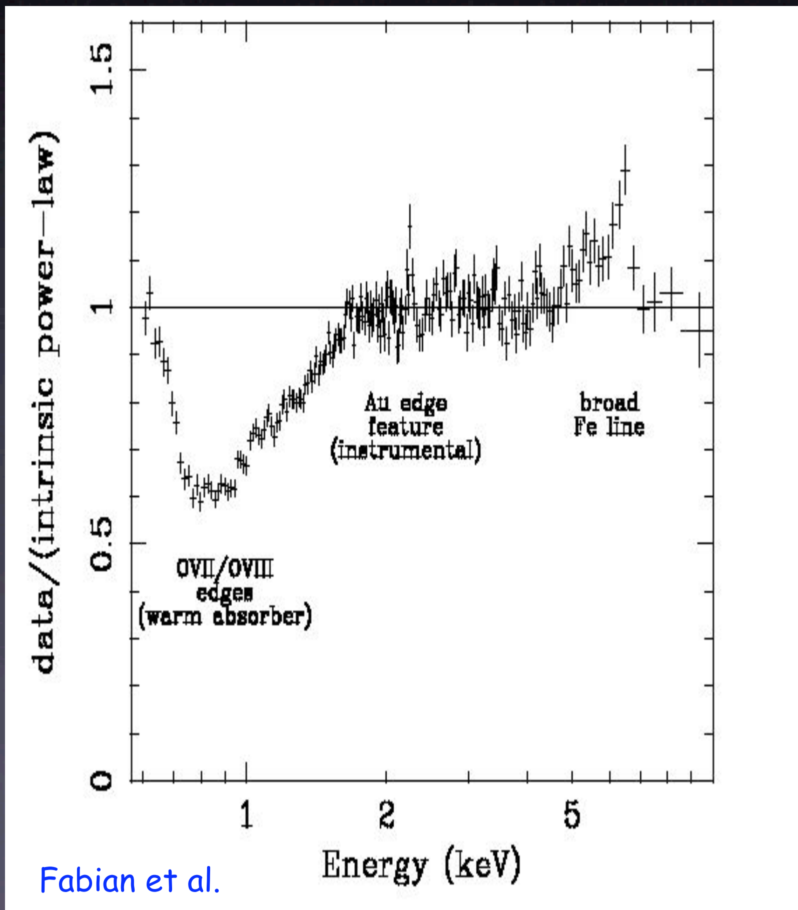
Example based on lines detected in the Chandra HETGS

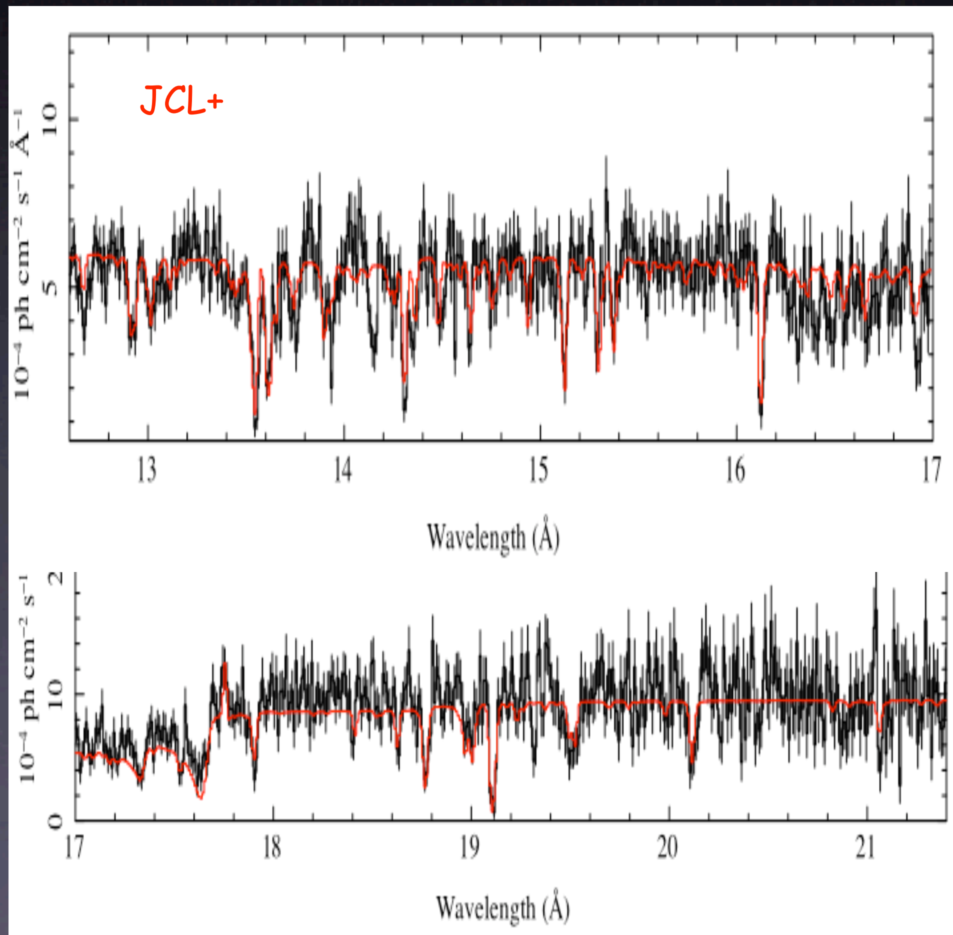
X-ray Spectroscopy in the 21st Century era of Chandra and XMM-Newton high spectral resolution instruments

X-ray Spectroscopy
Past and Present

ASCA SIS (R ~ 10 - 50)

Chandra HETGS (R ~ 200 - 1000)





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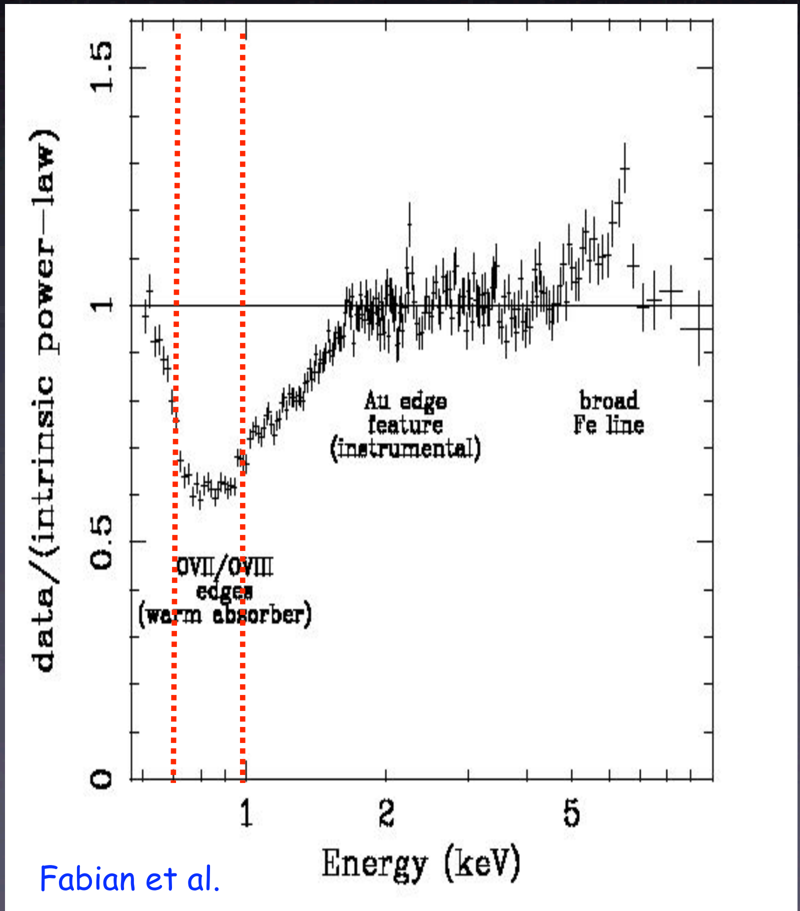
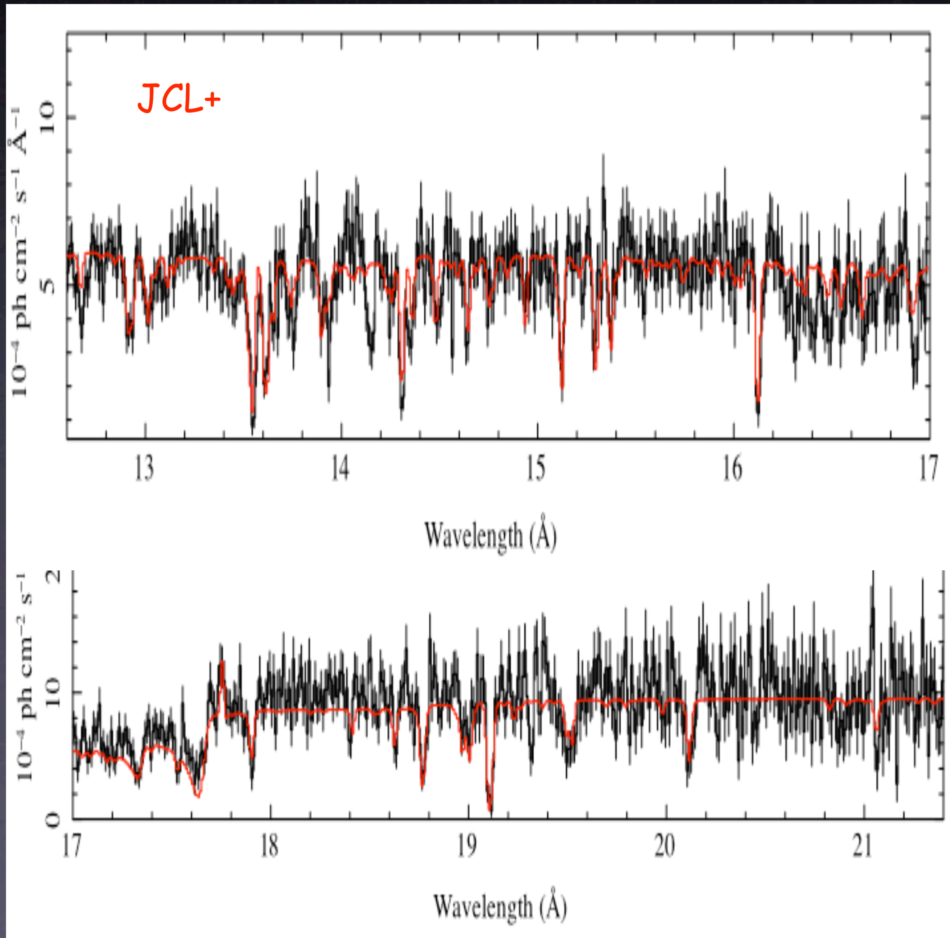
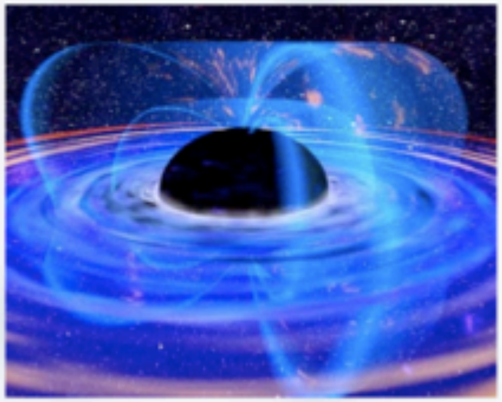


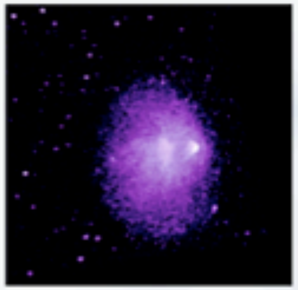


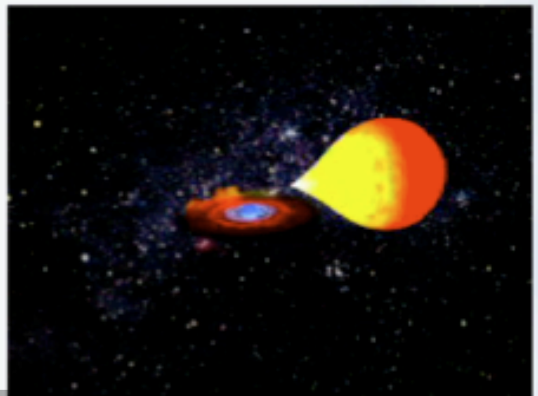
There are lots of Physics in the lines

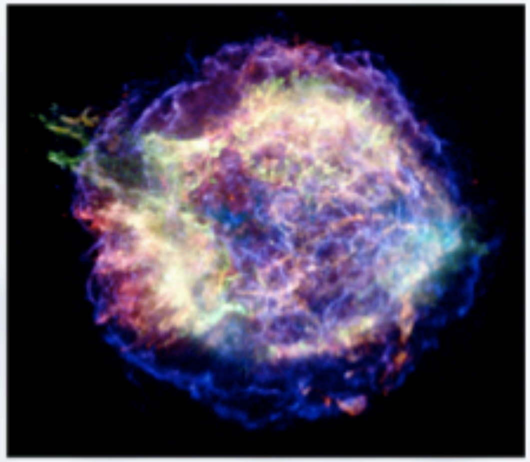
Spectrum provides precise information on ‘local’ conditions in the plasma

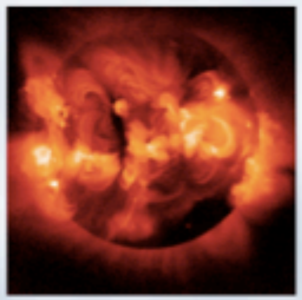
element, ionization stage, ionization mechanism, temperature, density,
degree of relaxation and past history,
velocities (thermal, turbulent, bulk, nonthermal), ***E*** and ***B*** fields, ...











no atomic physics @ >10 keV

Fig. from F. Paerels

The Electromagnetic Spectrum

Wave-Particle Duality: **$E = h\nu = hc/\lambda$**

Light waves = fluctuation of E&B fields due to atomic & molecular interactions

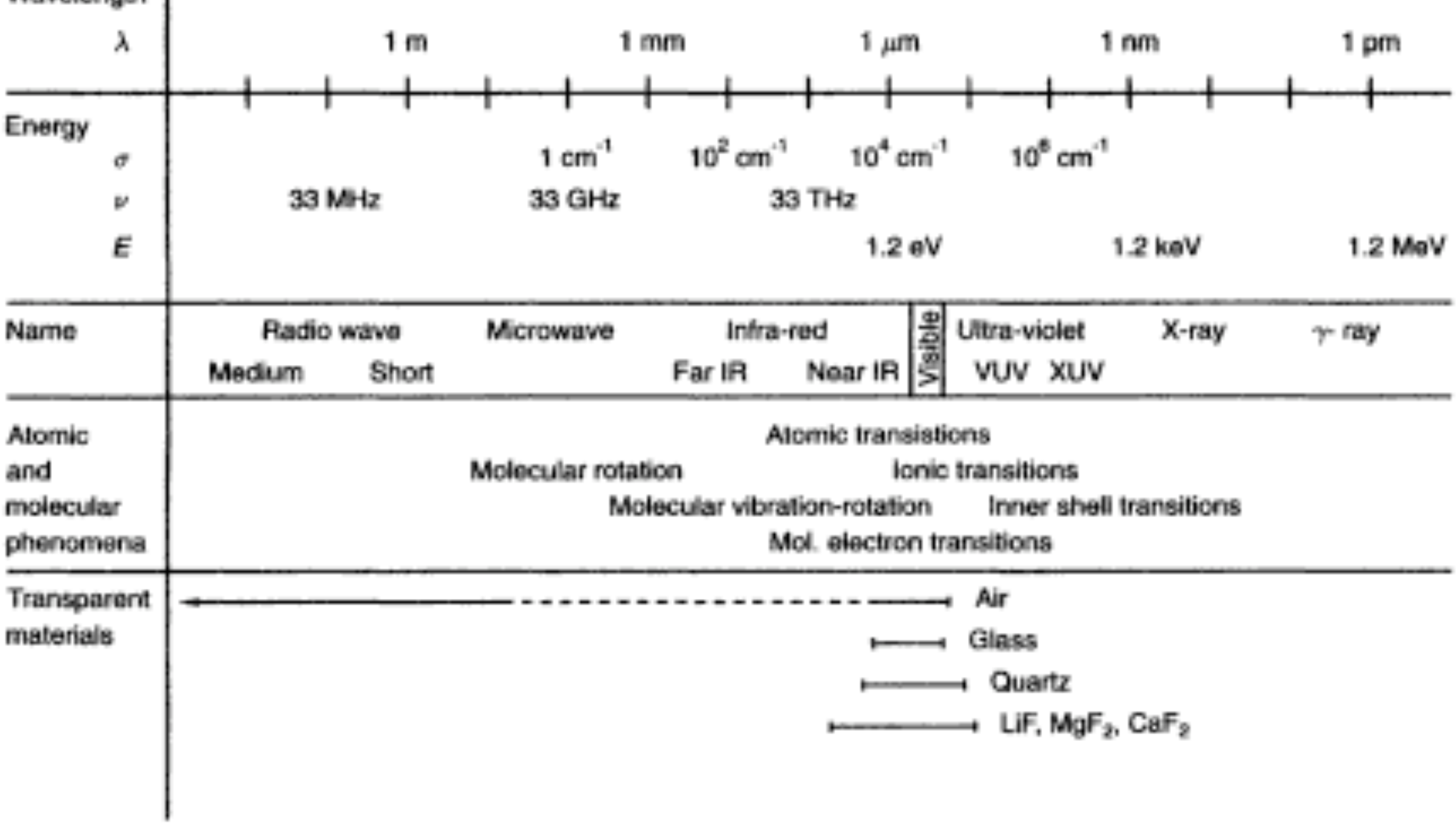


Figure from “Spectrophysics: Principles & Applications” by Thorne, Litzen, Johansson

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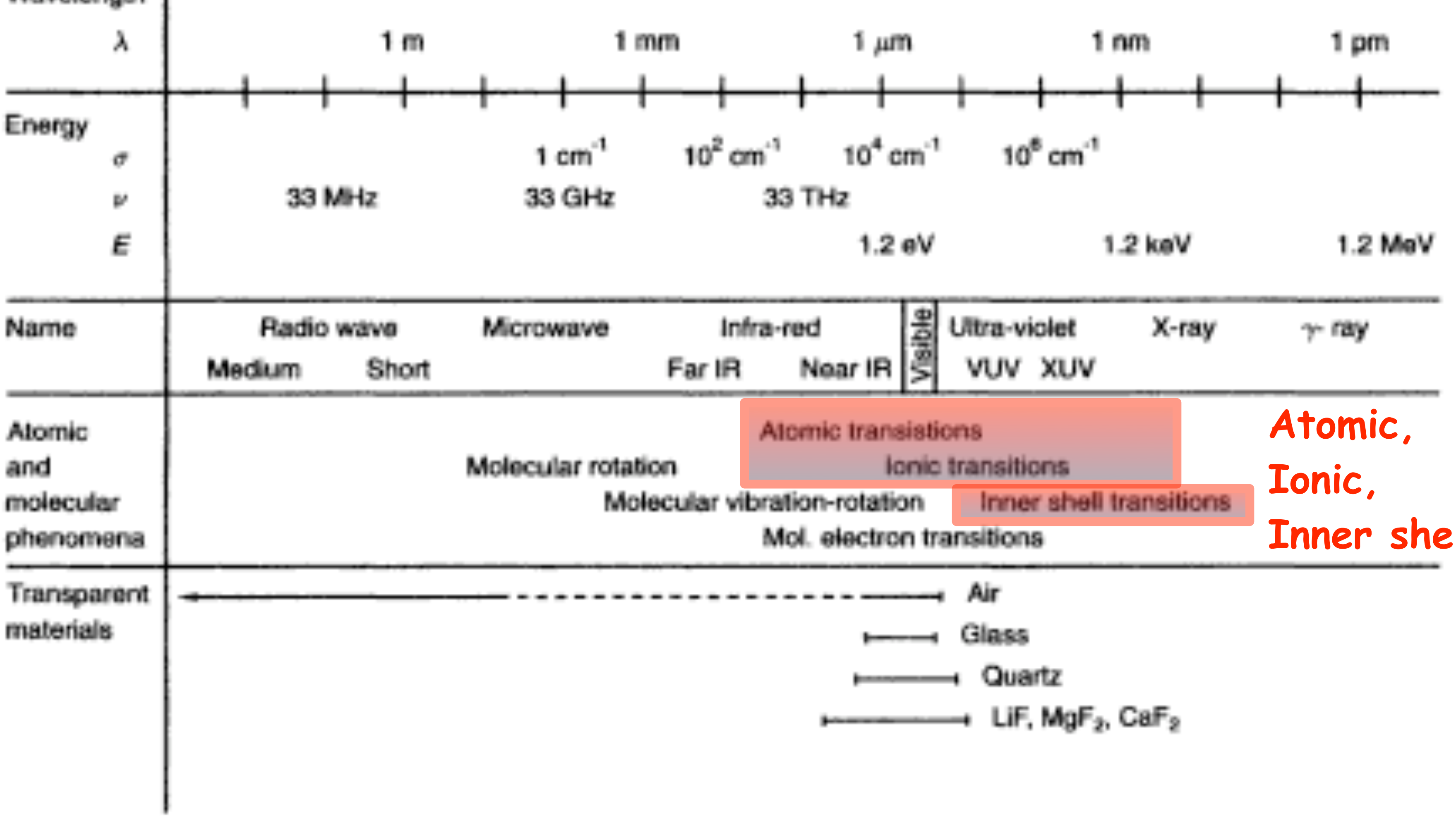
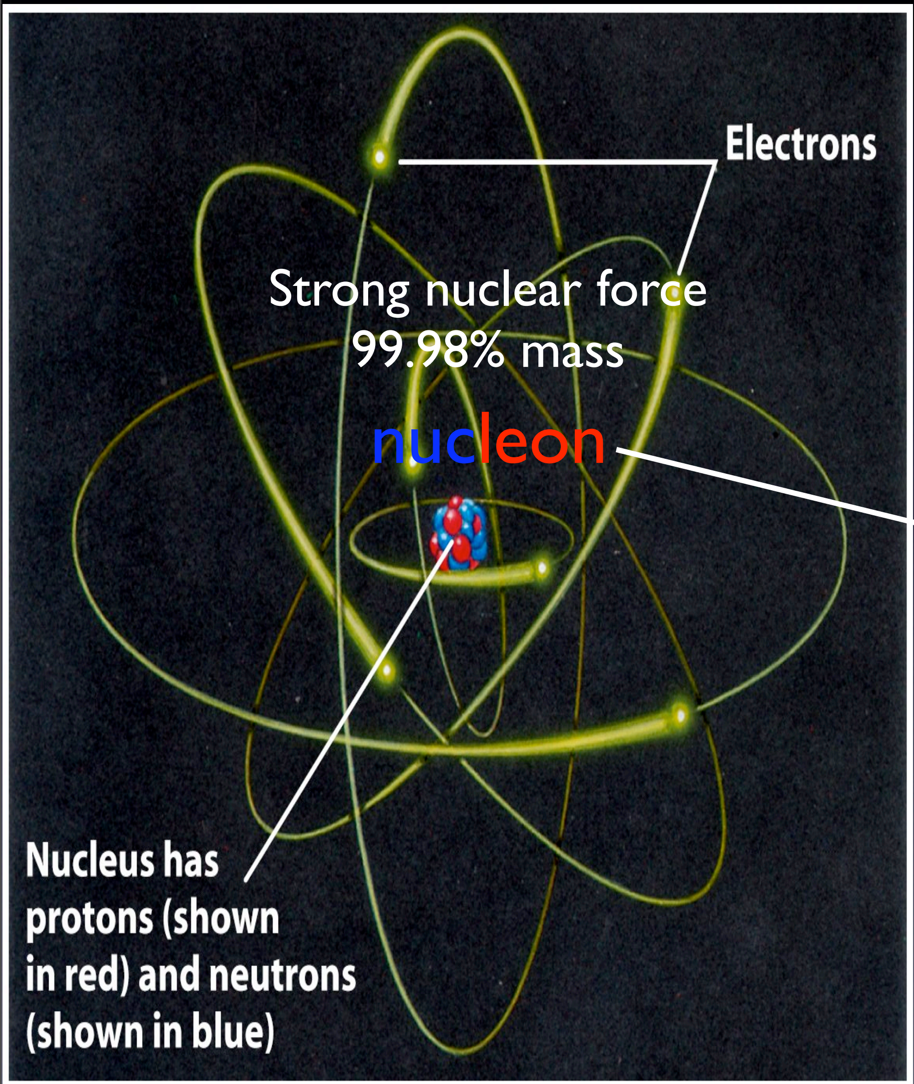


Atomic,
Ionic,
Inner shell

Figure from "Spectrophysics: Principles & Applications" by Thorne, Litzen, Johansson

The Structure of the Atom

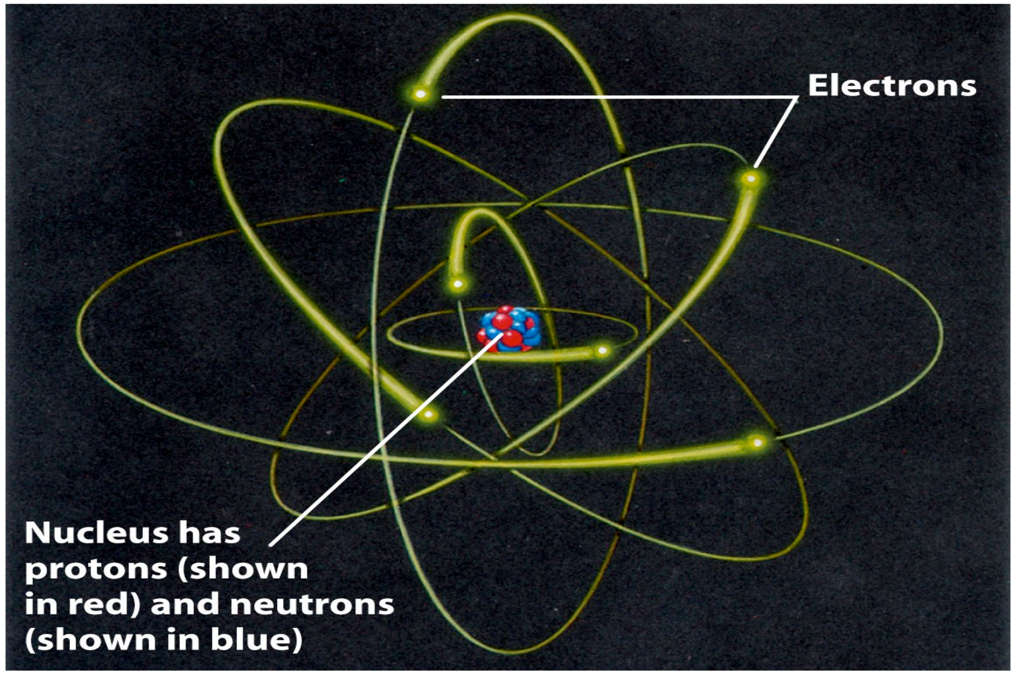
Terminology for this lecture



Smallest component of an element having properties of that element

- subatomic particles @ nucleus
  - neutron: n^0
  - proton: p^+ = Atomic# Z
- elementary particle surrounding nucleus
  - electron: e^-

Terminology: The Structure of the Atom



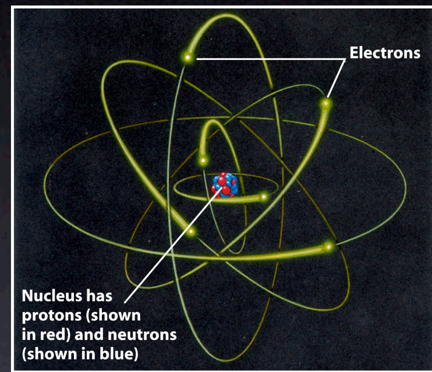
ATOM: smallest component of an element having properties of that element, made up of subatomic particles nucleons= $p^+ + n^0$ surrounded by e^-

- **Ionization**: physical process by which an e^- is removed (or added by capture) to an atom
  - net (+) via absorption
  - net (-) via collisions
- **Ion**: atom with:
  - $\geq$ 1e^- missing -> net (+)
  - $\geq$ 1e^- added -> net (-) (less common)
- **Molecules**:
  - > 1 atom forming bond

Atomic Processes in Hot Plasmas

Plasma constituents: electrons, ions, photons

Plasma physics Interests: ion interactions with an electron or photon, which result in changes either in the state of the ionization or excitation of the interacting ion



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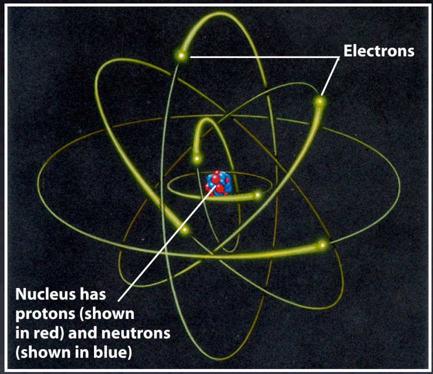

ions

electrons

photon (light)

ELECTRONS are accelerated by close approaches to IONS

As the temperature rises, the PHOTON (light) production increases

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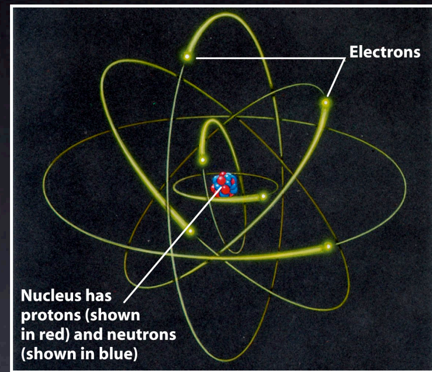

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Classification of Ionic Processes

(there are other schemes)

* ✳ Spontaneous ion decay
* ✳ Photon-ion Processes
* ✳ Electron-ion interactions
* ✳ Ion-ion interactions (chg xchg)
* ✳ Photon-electron processes

Atomic Processes in Hot Plasmas

Direct Process	Inverse Process
Spontaneous Decay	Resonant Photoabsorption
Autoionization	Dielectron Recombination
Photoionization	Radiative Recombination
Electron Impact Ionization	3-body recombination (electron impact recombination)
Electron Impact Excitation	Electron Impact De-excitation
Bremsstrahlung	Inverse Bremsstralung

Photon-Ion Interaction

Direct Process	Inverse Process
Spontaneous Decay	**Resonant Photoabsorption**
Autoionization	Dielectron Recombination
Photoionization	Radiative Recombination
Electron Impact Ionization	3-body recombination (electron impact recombination)
Electron Impact Excitation	Electron Impact De-excitation
Bremsstrahlung	Inverse Bremsstralung

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Electron-Ion Interaction

Direct Process	Inverse Process
Spontaneous Decay	Resonant Photoabsorption
Autoionization	Dielectron Recombination
Photoionization	Radiative Recombination
Electron Impact Ionization	3-body recombination (electron impact recombination)
Electron Impact Excitation	Electron Impact De-excitation
Bremsstrahlung	Inverse Bremsstralung

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No particle interaction

Direct Process	Inverse Process
Spontaneous Decay	Resonant Photoabsorption
Autoionization	Dielectron Recombination
Photoionization	Radiative Recombination
Electron Impact Ionization	3-body recombination (electron impact recombination)
Electron Impact Excitation	Electron Impact De-excitation
Bremsstrahlung	Inverse Bremsstralung

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Photon-Electron Interaction (free-free) (Continuum Spectrum - no lines)

Direct Process	Inverse Process
Spontaneous Decay	Resonant Photoabsorption
Autoionization	Dielectron Recombination
Photoionization	Radiative Recombination
Electron Impact Ionization	3-body recombination (electron impact recombination)
Electron Impact Excitation	Electron Impact De-excitation
Bremsstrahlung	**Inverse Bremsstralung**

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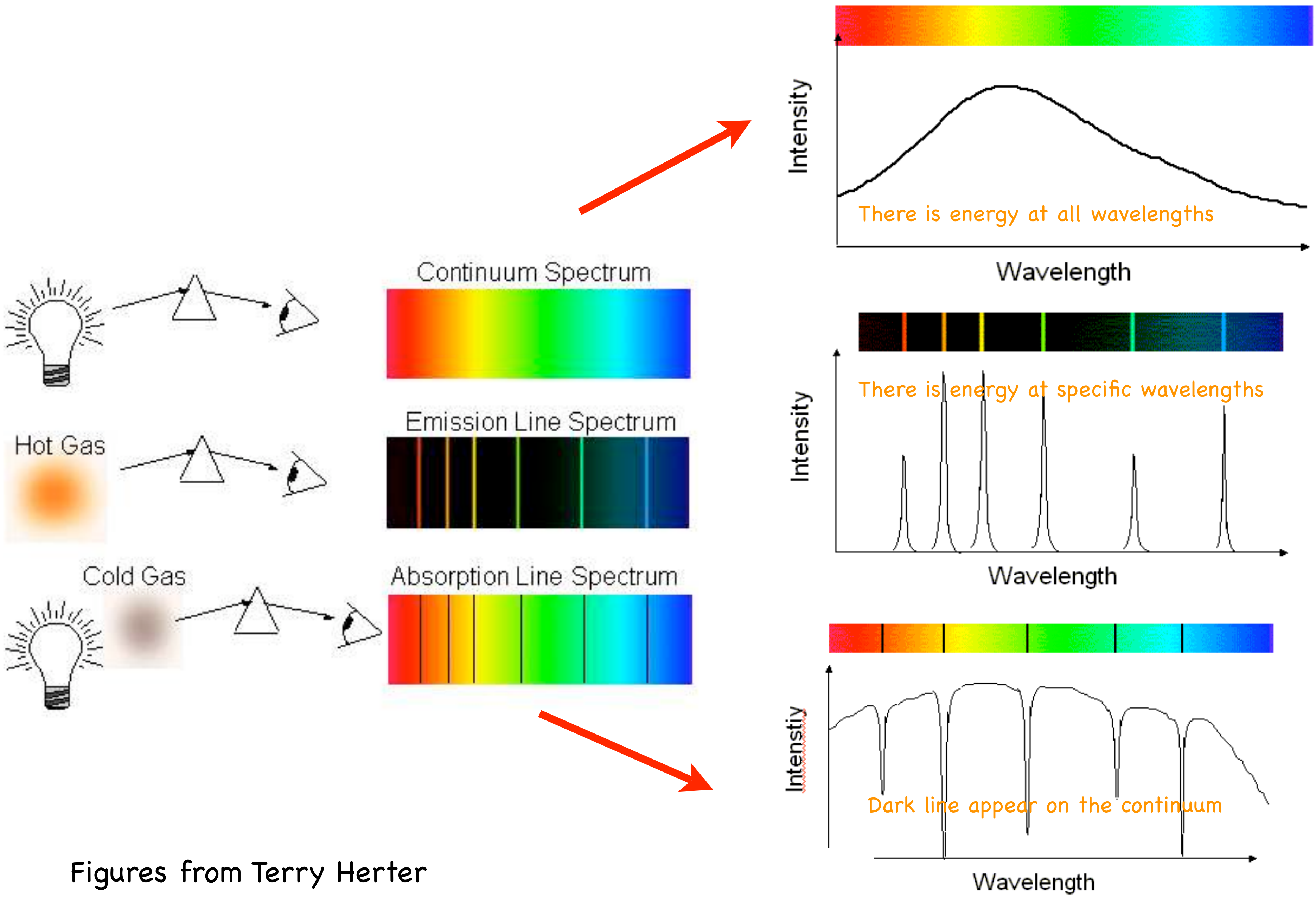
And now for some words on Proton collisions.

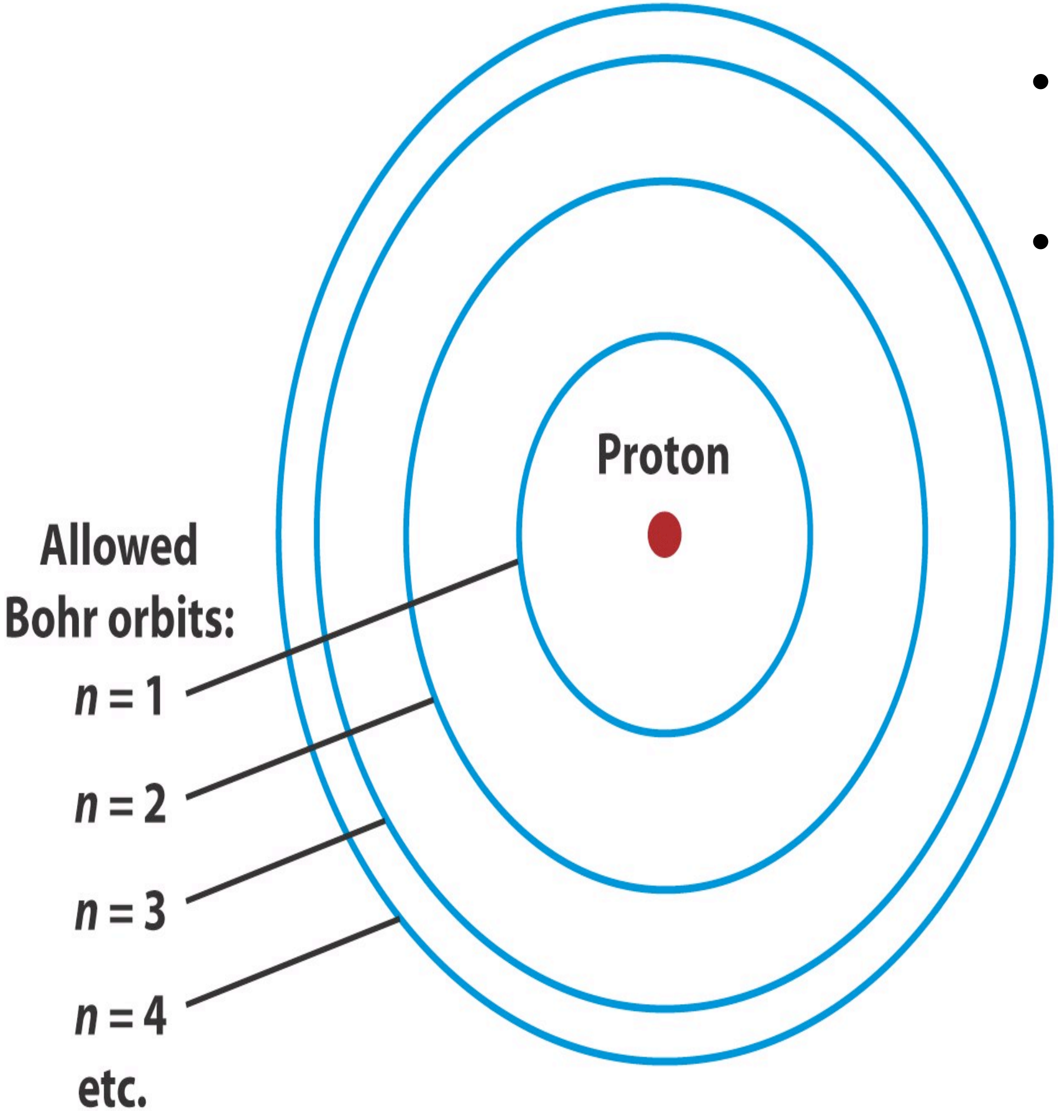
In equilibrium, since protons are 1836x more massive than electrons, their speed will be ~43x slower than that of electrons. As a result, the collision rate <nσv> for protons will be much lower. In addition, protons are positively charged, as are ions, so that also means small impact parameter (high momentum transfer) collisions are suppressed.

As a result, proton collisions can *usually* be ignored - except for low-lying transitions within an ion's ground state, which can be excited by proton collisions.



Figures from Terry Herter

Some Quantum Mechanics Laws



- Strict Laws governing quantization of energy levels
- Arrangement of permitted orbits depends primarily on charge of nucleus which depend on number of protons
  - each element (and their isotopes) have similar orbits
  - different elements have different orbits
  - ionized atoms have different orbits from unionized ones

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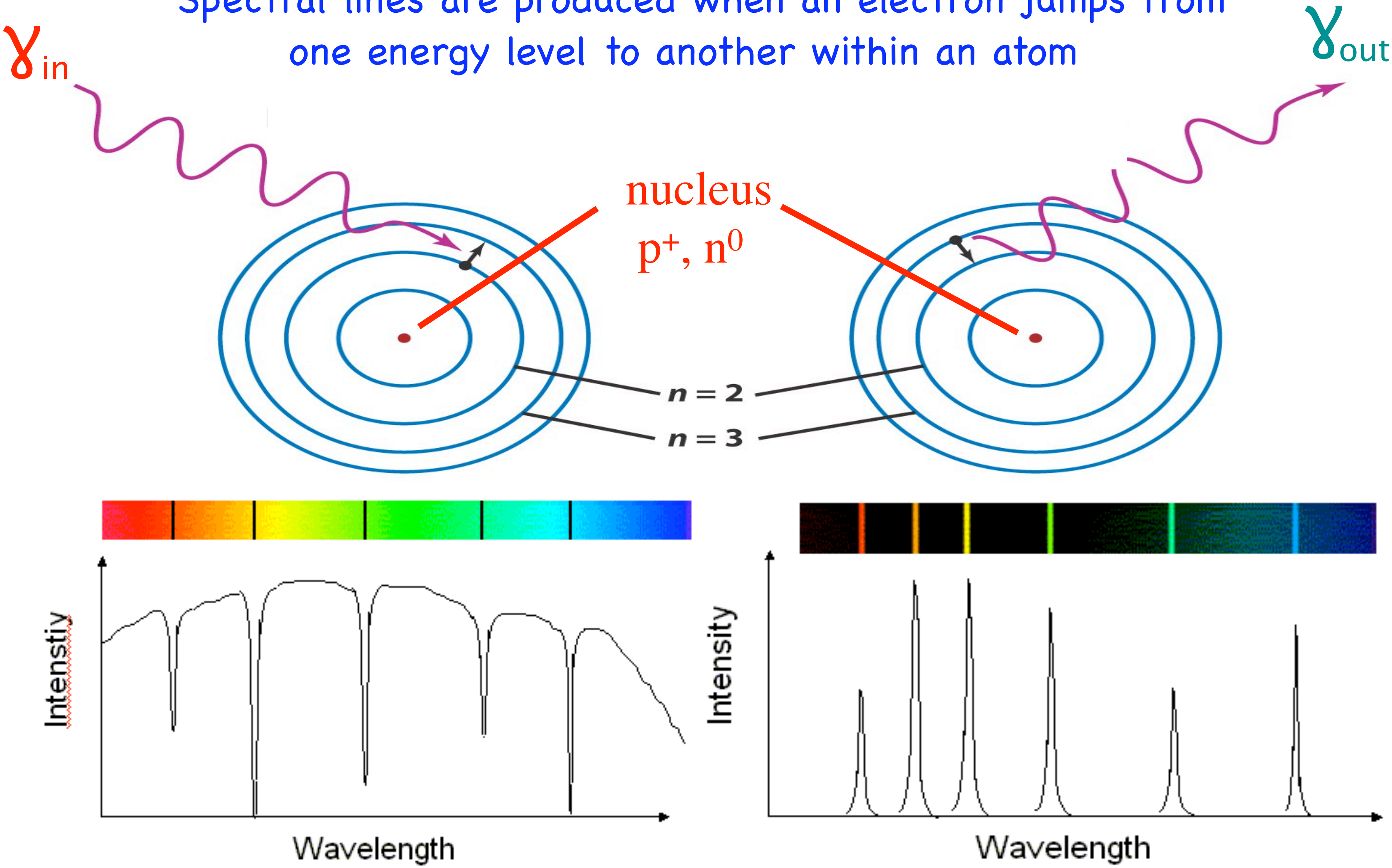
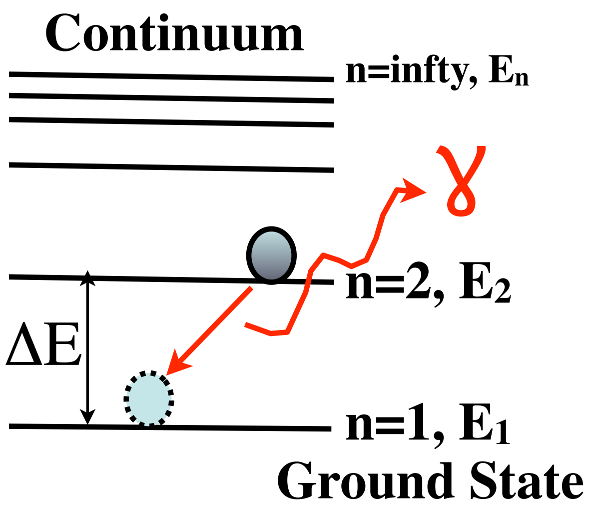
Absorption / Emission

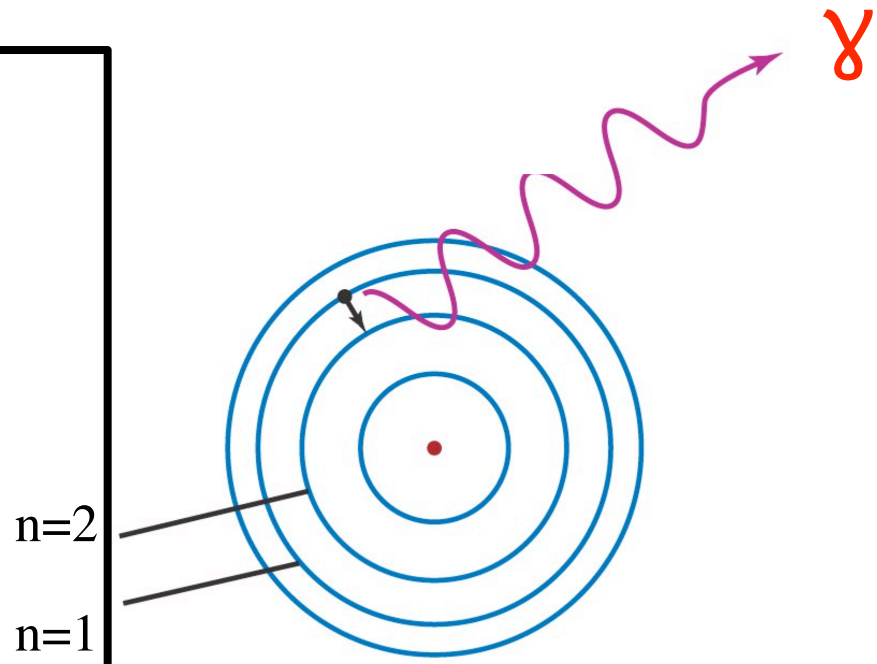
depends on electron transitions

Spectral lines are produced when an electron jumps from one energy level to another within an atom



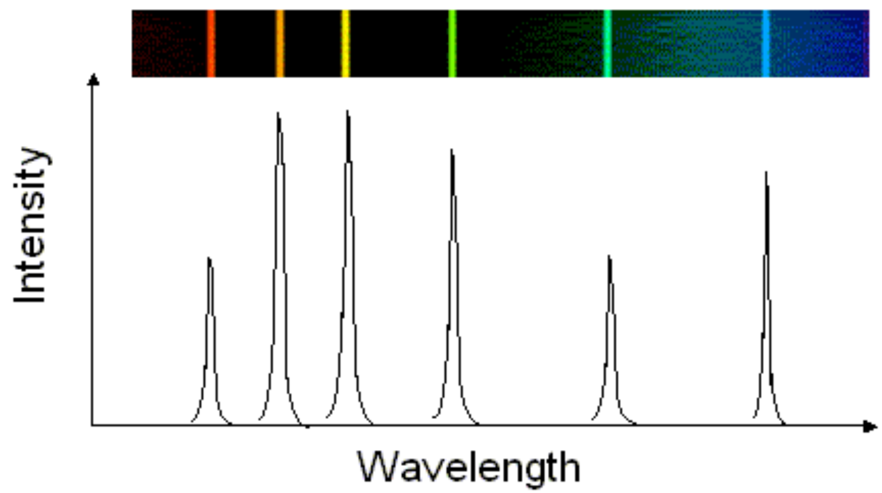
Emission: light bands



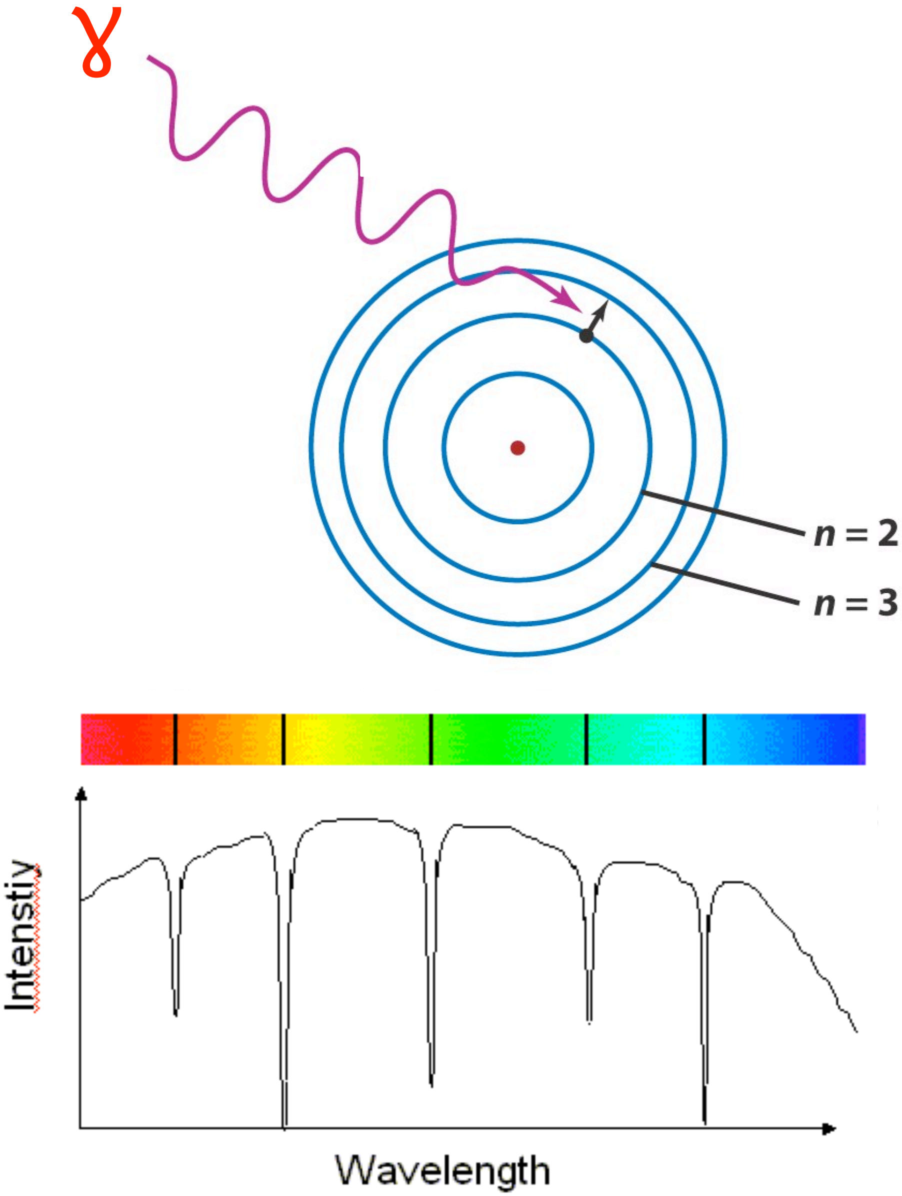


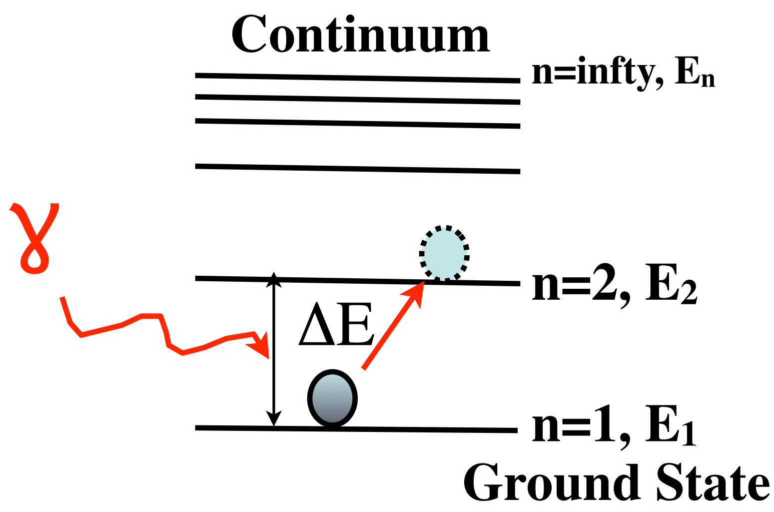
Atom in excited state, decays to lower stable state

emits photon = $|E_n - E_{n+1}|$



Absorption: dark bands

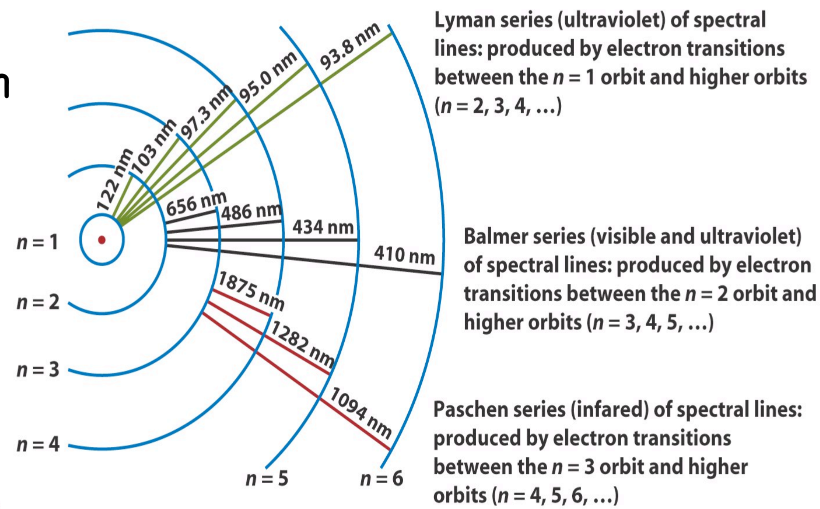


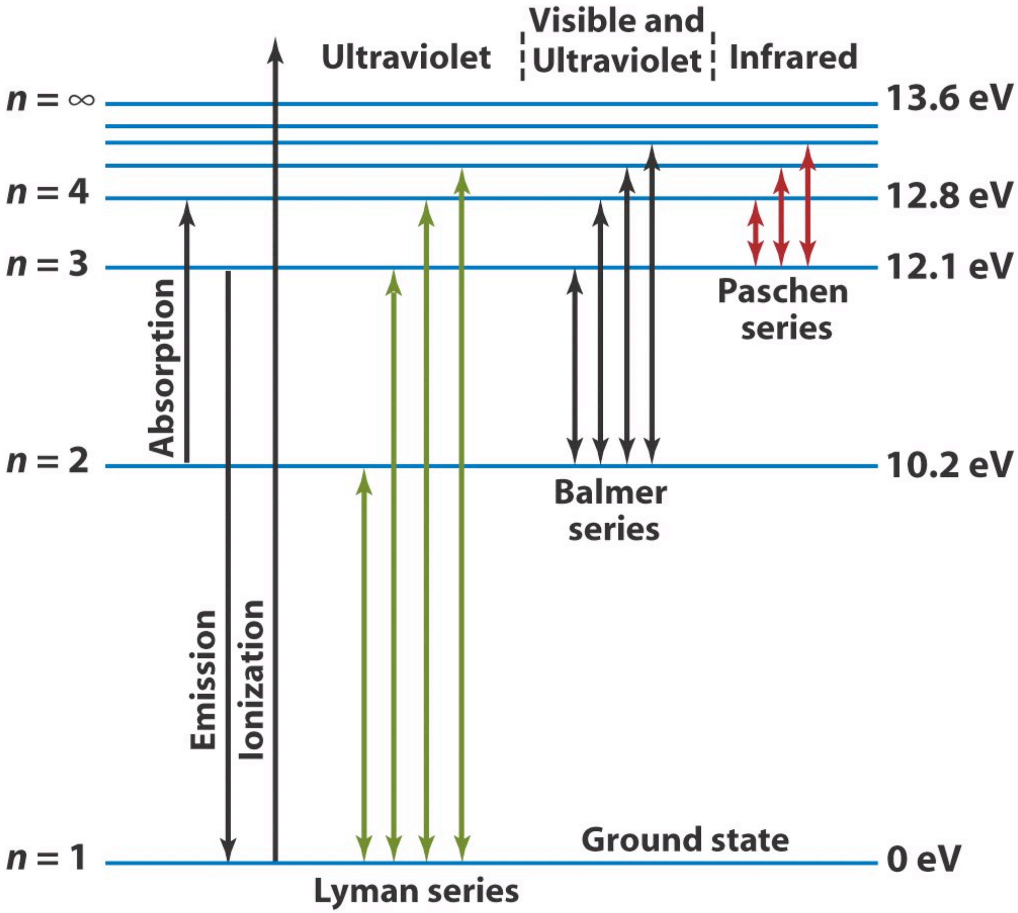


Atom in stable state:
absorbs photon = $|E_n - E_{n+1}|$

Photoelectron goes to higher quantum state

Bohr's Energy Level Diagram for Hydrogen
but concept for transition diagrams hold





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Fermi's Golden Rule

Transition Rate / Cross section = a measure of the number of reactions undergone by one particle per unit time / probability for transition

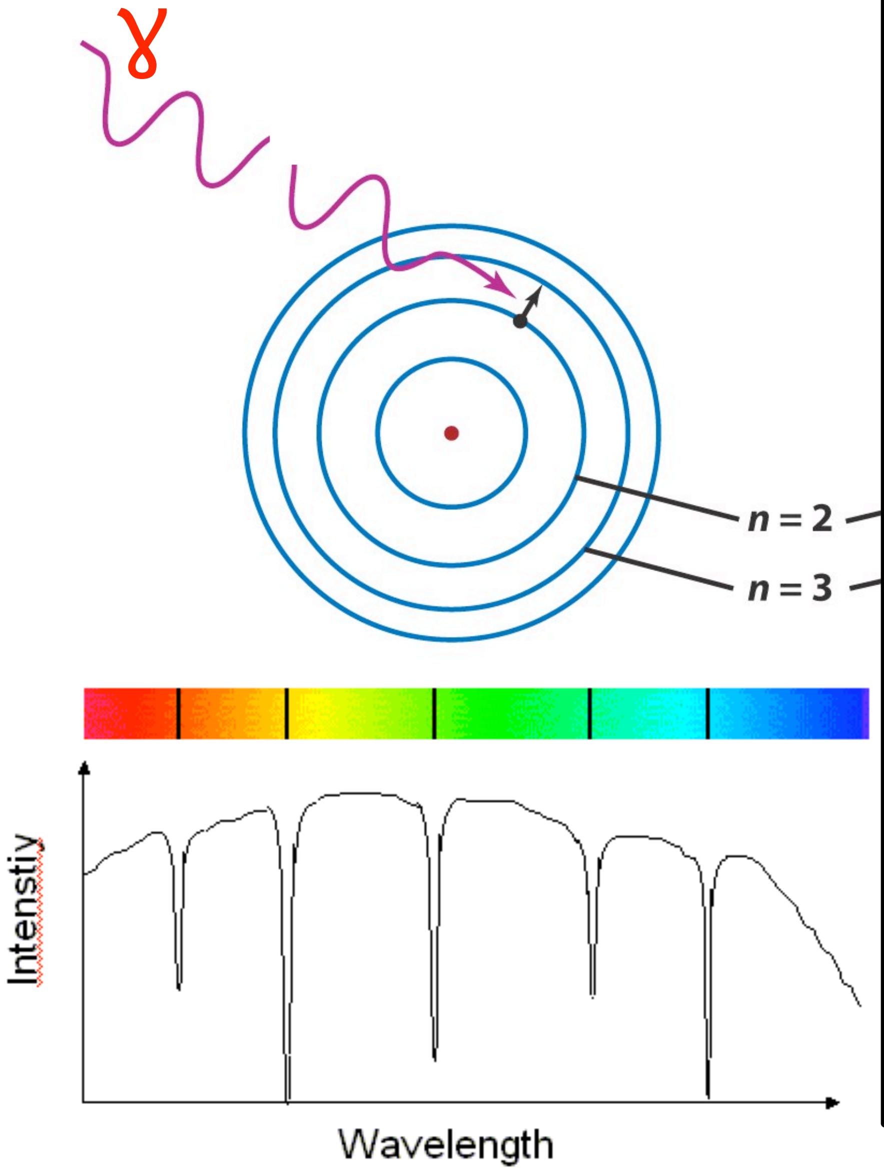
final state of particle

$$\mu(E) \propto |<i|\mathcal{H}|f>|^2$$

initial state of particle

Hamiltonian of the interaction

Absorption



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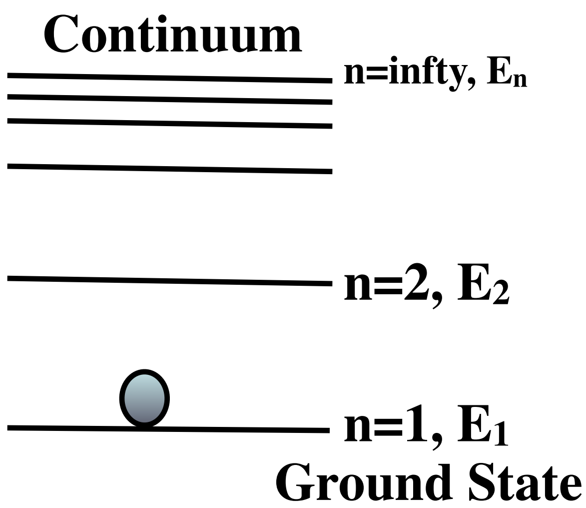
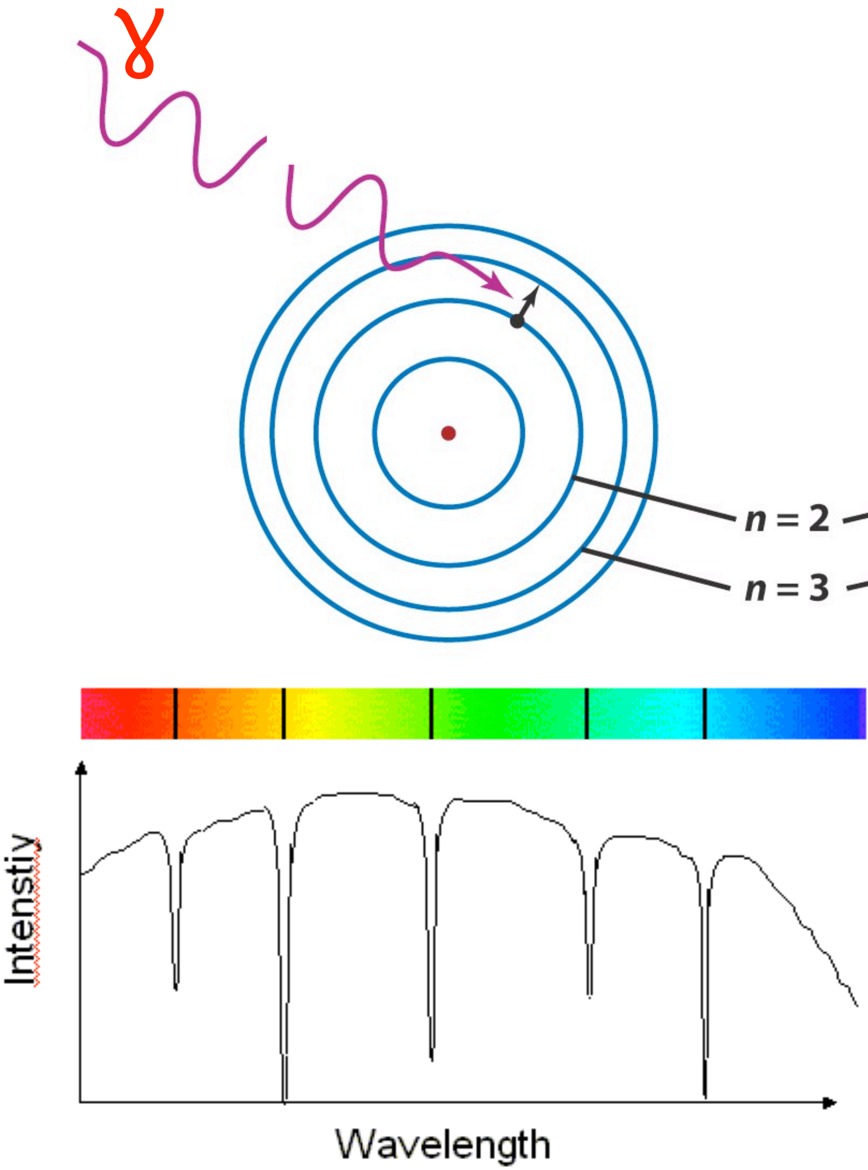
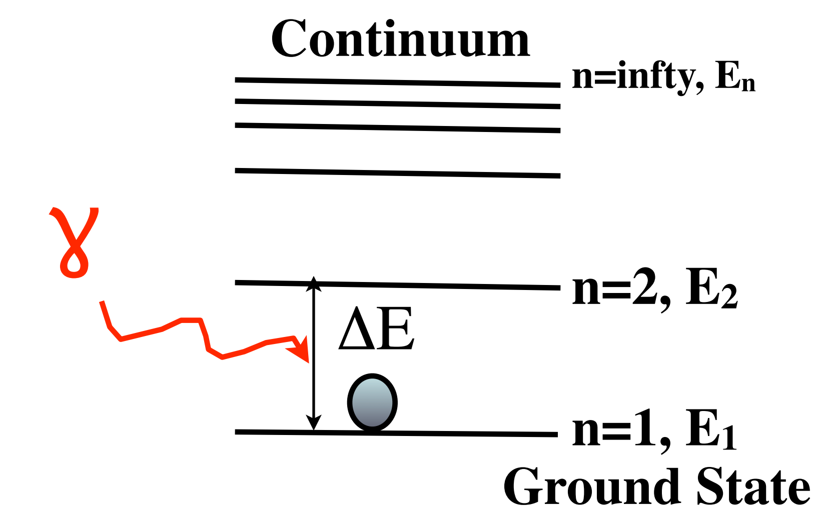


Atom **absorbs** photon = $|E_n - E_{n+1}|$: $A_l \rightarrow A_u$

Absorption



$$\mu(E) \propto |\langle i | \mathscr{H} | f \rangle|^2$$



$\langle i |$ X-ray, core e-, no photoelectron

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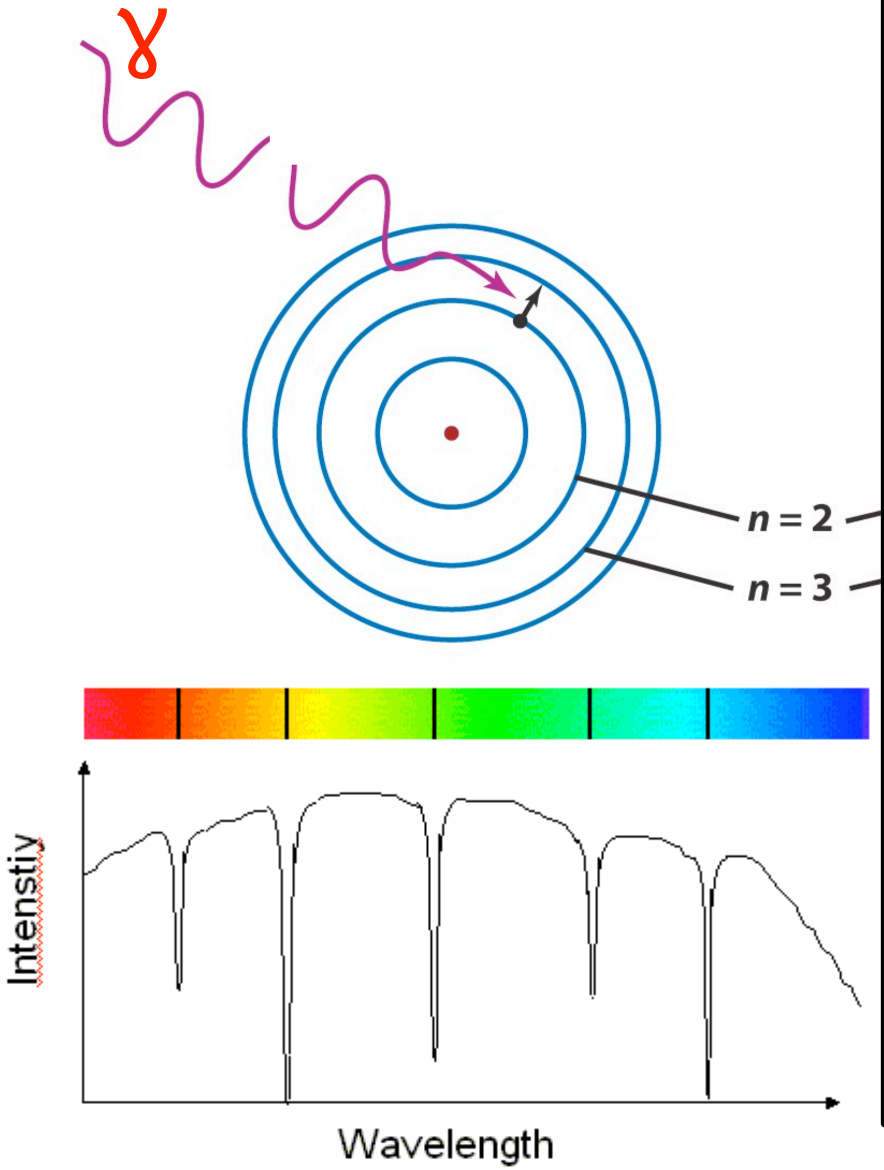
Absorption



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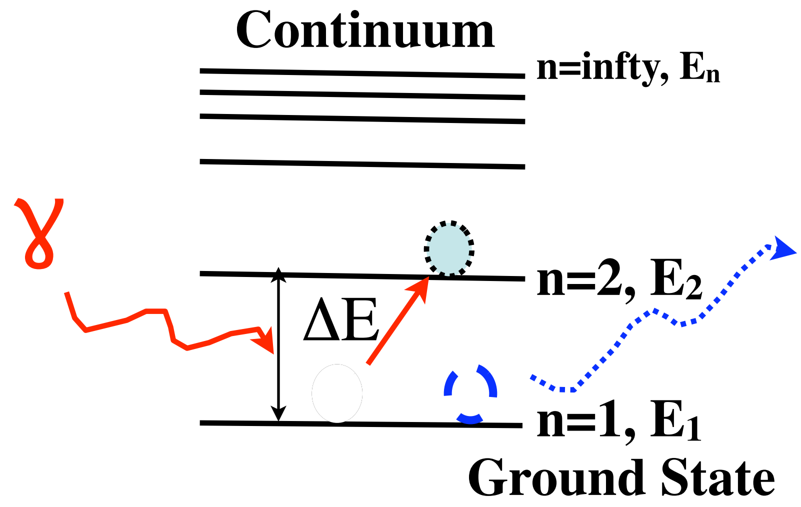
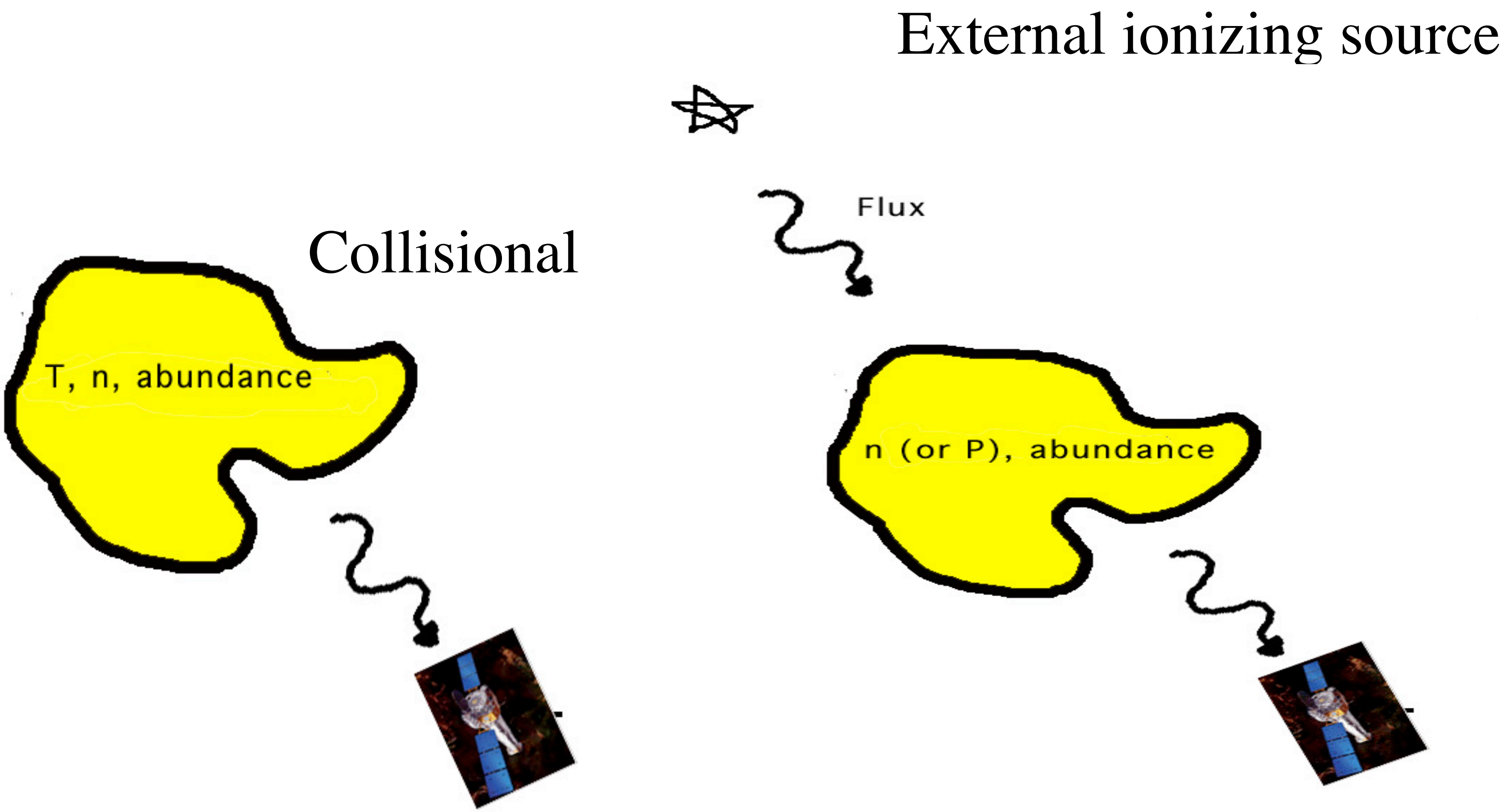


$< i |$ X-ray, core e-, no photoelectron

$| f >$ no X-ray, core hole, photoelectron

Atom **absorbs** photon = $|E_n - E_{n+1}|$: $A_l \rightarrow A_u$

Plasmas in Astrophysics of X-ray Interest



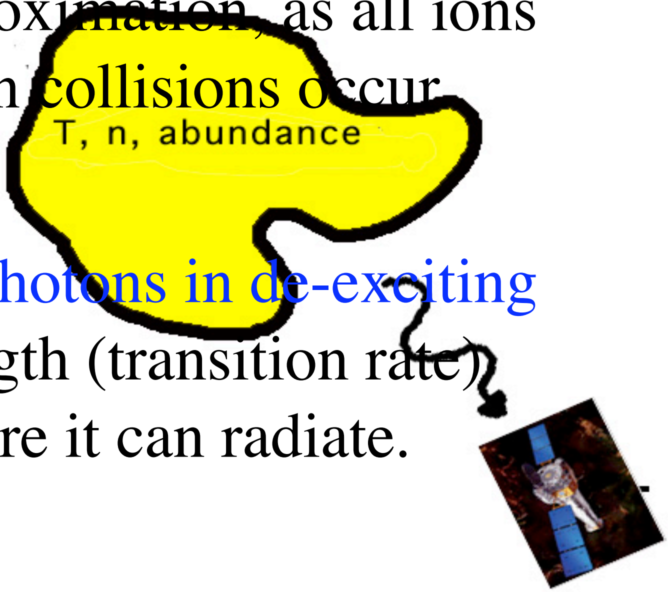
- $k_B T_e \sim$ Ionization energy of plasma ions
- $k_B T_e <<$ Ionization energy of plasma ions

Collisional (Thermal) Plasma

Astrophysical **collisional** plasmas come in two types:

- Coronal / Nebular: $N_e < 10^{14} - 10^{16}\ \text{cm}^{-3}$
- Collisional-Radiative: $10^{14}\ \text{cm}^{-3} < N_e < 10^{27}\ \text{cm}^{-3}$

In the more common Coronal (or Nebular) plasma, collisions excite ions but rarely de-excite them; the decay is radiative. This is also called the "ground-state" approximation, as all ions are assumed to be in the ground-state when collisions occur.

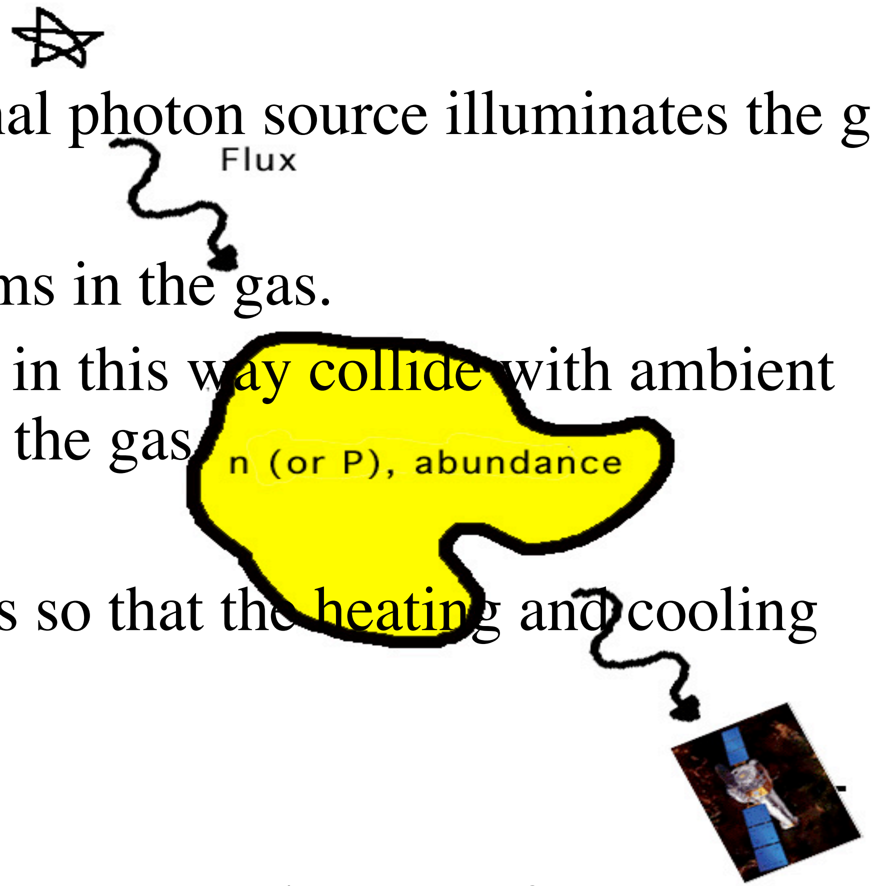


In a CR plasma, collisions compete with photons in de-exciting levels; a level with a small oscillator strength (transition rate) value may be collisionally de-excited before it can radiate.

Photoioniized Plasma

What happens when an external photon source illuminates the gas?

- The photons ionize the atoms in the gas.
- The photoelectrons created in this way collide with ambient electrons (mostly) and heat the gas
- The gas cools by radiation
- The gas temperature adjusts so that the heating and cooling balance



In a photoionized gas the *temperature* is not a free parameter
and
The *ionization balance* is determined by the shape and strength of the *radiation field*

Parameter definitions:

$$\xi \equiv \frac{L}{n_e R^2}$$ Tarter, Tucker & Salpeter (1969)

$$U_x \equiv \frac{N_X}{4\pi R^2 nc}$$ Davidson (1974)

$$\Gamma \equiv \frac{L_X(> 13.6\ \mathrm{eV})}{8\pi R^2 nc}$$ Kwan & Krolik (1981)

$$\Xi \equiv \frac{L}{4\pi n_e ckTR^2}$$ Krolik, McKee & Tarter (1982)

$$U_1 \equiv \frac{N}{4\pi R^2 nc}$$ Netzer (1994)

where:

$$L \equiv \int_{13.6\ \mathrm{eV}}^{\infty} L(E)\,dE \qquad N \equiv \int_{13.6\ \mathrm{eV}}^{\infty} L(E)\frac{dE}{E} \qquad N_X \equiv \int_{100\ \mathrm{eV}}^{\infty} L(E)\frac{dE}{E}$$

Highlights: Coronal vs. Photoionized

- Coronal Gas:
  - need $kT_e \sim \Delta E$ to collisionally excite lines.
- Photoionized Gas:
  - External ionizing source
  - Temperature lower for same ionization than coronal, $T \sim 0.1\, E_{th}/k$
    - temperature not a free parameter; depends on spectral shape
  - Excitation is often by recombination cascade
  - Also get recombination continua (RRCs) due to recombination by cold electrons directly to the ground state. The width of these features is directly proportional to temperature
  - Due to the democratic ionization balance, it is more likely that diverse ions such as N VII, O VIII, Si XIV can coexist and emit efficiently than it would be in a coronal gas
  - Inner shell ionization and fluorescence is also important in gases where the ionization state is low enough to allow ions with filled shells to exist.

Ionization

Ionization is a relatively simple process, with three main channels:

Photoionization: $\gamma + I \rightarrow I^+ + e^-$

Collisional ionization: $e^- + I \rightarrow I^+ + 2e^-$

Inner-shell ionization: $\gamma, e^- + I \rightarrow I^{*+} + 2e^- \rightarrow I^+ + e^-, \gamma$

Photoionization and collisional ionization have been measured in the lab and theoretical calculations are relatively straightforward, so little attention is paid to them now.

Plasmas in Astrophysics of X-ray Interest

	Photoionized	Coronal
Dominant ionization	Photoionization $h\nu$ +Z –>Z+1	Electron impact e^-+Z -> Z+1
Examples	Active galaxies(AGN) SNR H II regions	Stellar coronae Supernova remnant Clusters of galaxies
Spectral signature	Absorption,bound-free, bound-bound Emission: recombination	Emission lines, Δn= 0,1,2 favored

Table from R. Smith

There are lots of Physics in the lines

- Line position : ion identification
- Line shifts: dynamics, e.g. inflow, outflow
- Line strengths
  - ionic column : e.g. N_{OVII}, N_{NeX}, N_{FeXXVI} ...
  - degree of ionization : e.g. H-like/He-like
  - temperature, density
- Line widths : e.g. turbulence, GR

There are lots of Physics in the lines

First, a small digression

The isoelectronic sequence

(a slight digression on terminology)

- All ions with the same number of electrons have similar internal structure
  - H ~ H-like CVI (+5), OVIII (+7), NeX, MgXII, Si XIV
  - He ~ He-like CV (+4), OVII (+6), NeIX, MgXI, SiXIII ...
  - to 1st order, electronic states differ only by scaling factor:
    - energies larger by Z^2_{eff}
    - radii smaller by $1/Z_{eff}$

Ions of Importance in X-rays Emitting Plasmas

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H-like : All transitions of astrophysically abundant metals (C→Ni) are in the X-ray band. Lyα/Lyβ is a useful temperature diagnostic; Lyα is quite bright.

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Ions of Importance in X-rays Emitting Plasmas

H-like : All transitions of astrophysically abundant metals (C→Ni) are in the X-ray band. Lyα/Lyβ is a useful temperature diagnostic; Lyα is quite bright.

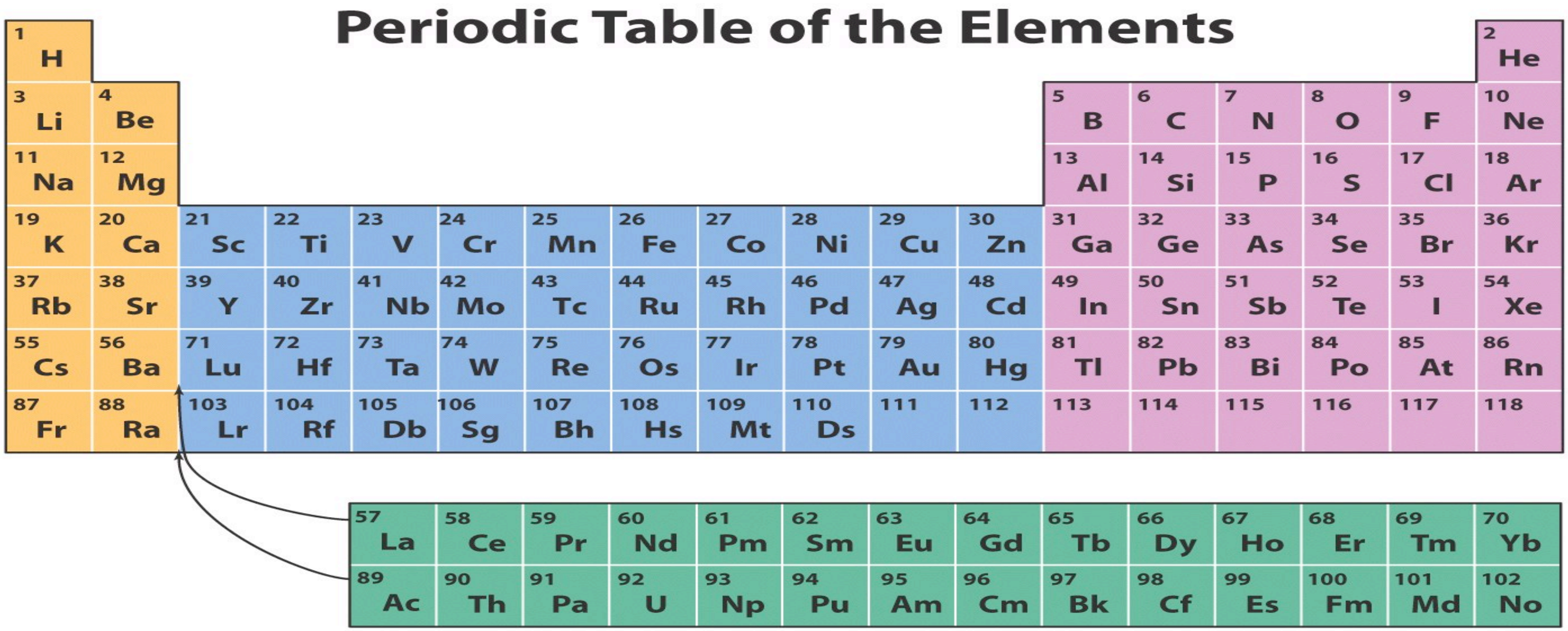
He-like: Δn≥1 transitions are all bright and in X-ray. The n=2→1 transitions have 4 transitions which are useful diagnostics, although R=300 required to separate them.

Ne-like: Primarily Fe XVII; two groups of bright emission lines at 15Å and 17Å; ionization state and density diagnostics, although there are atomic physics problems.

There are lots of Physics in the lines

- **Line position : ion identification**
- Line shifts: dynamics, e.g. inflow, outflow
- Line strengths
  - ionic column : e.g. N_{OVII}, N_{NeX}, N_{FeXXVI} ...
  - degree of ionization : e.g. H-like/He-like
  - temperature, density
- Line widths : e.g. turbulence, GR

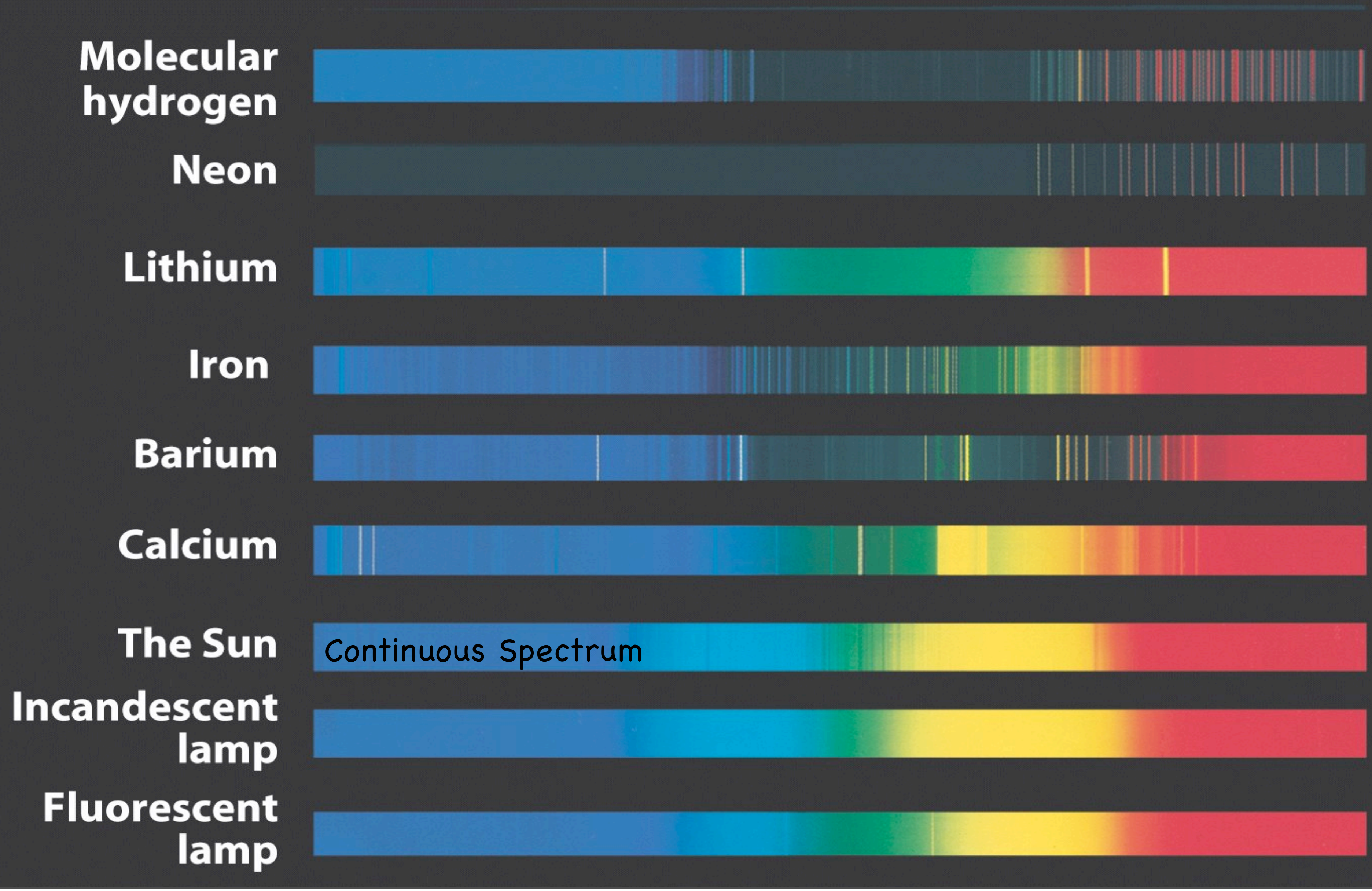
Recall Quantum Mechanics Laws



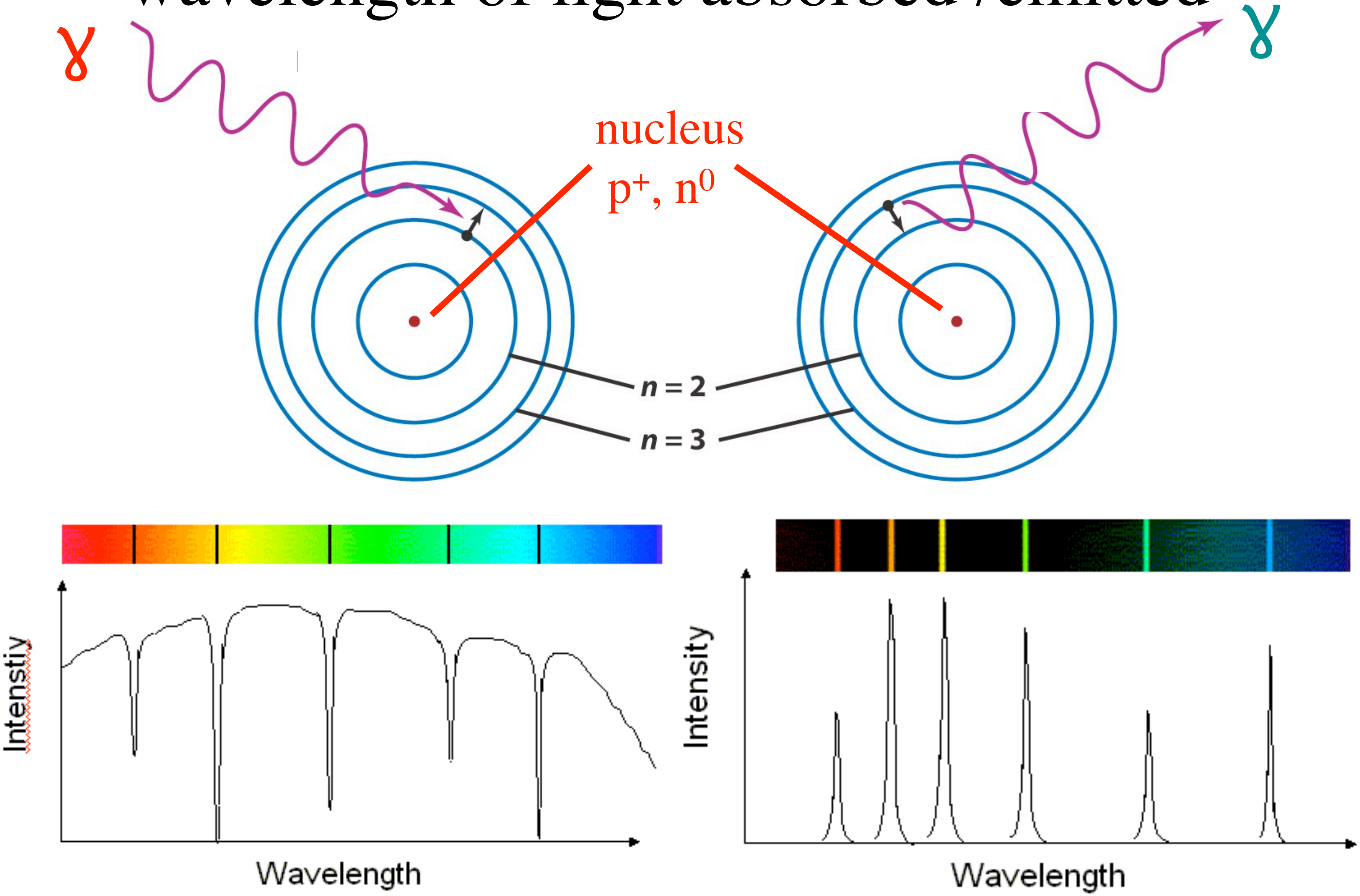
- Strict Laws governing quantization of energy levels
- Arrangement of permitted orbits depends primarily on charge of nucleus which depend on number of protons
  - each element (and their isotopes) have similar orbits
  - different elements have different orbits
  - ionized atoms have different orbits from unionized ones

Ions in Plasma : Line Position

Each element has unique set of permitted orbits depending on # of protons

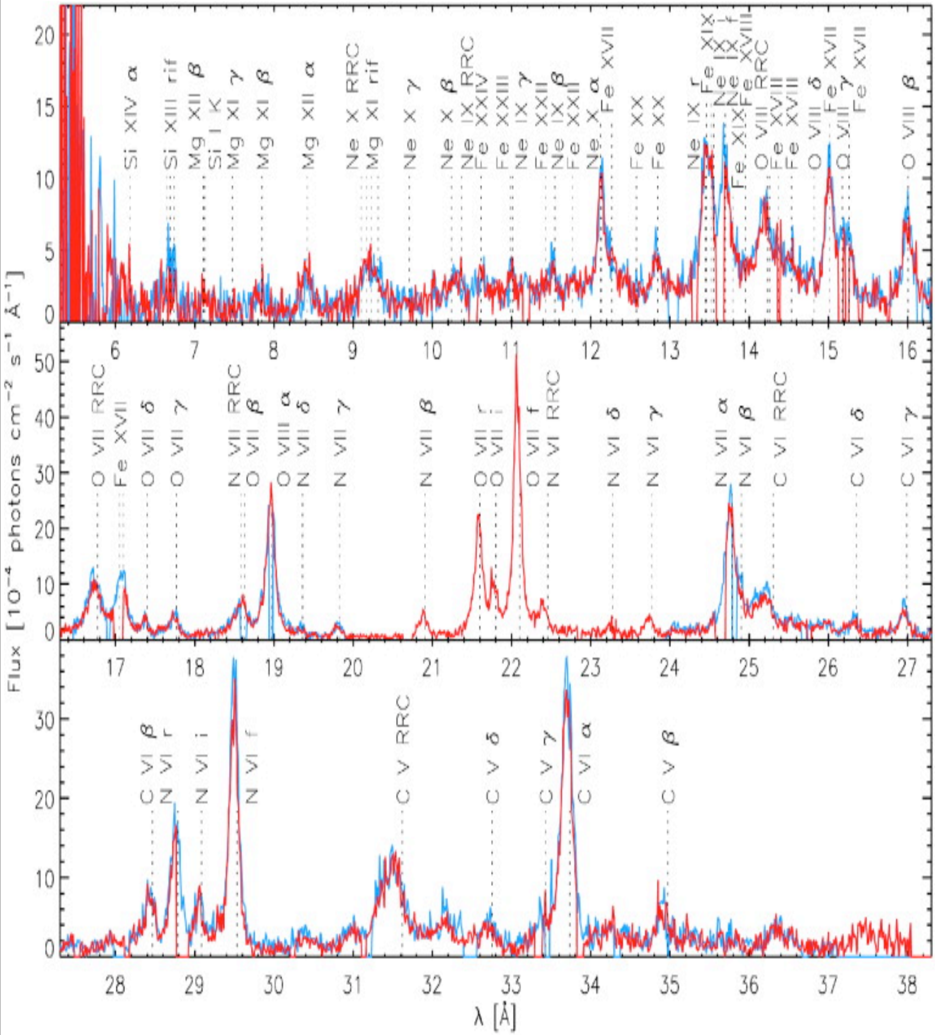


QM: Energy level of atoms determines wavelength of light absorbed /emitted

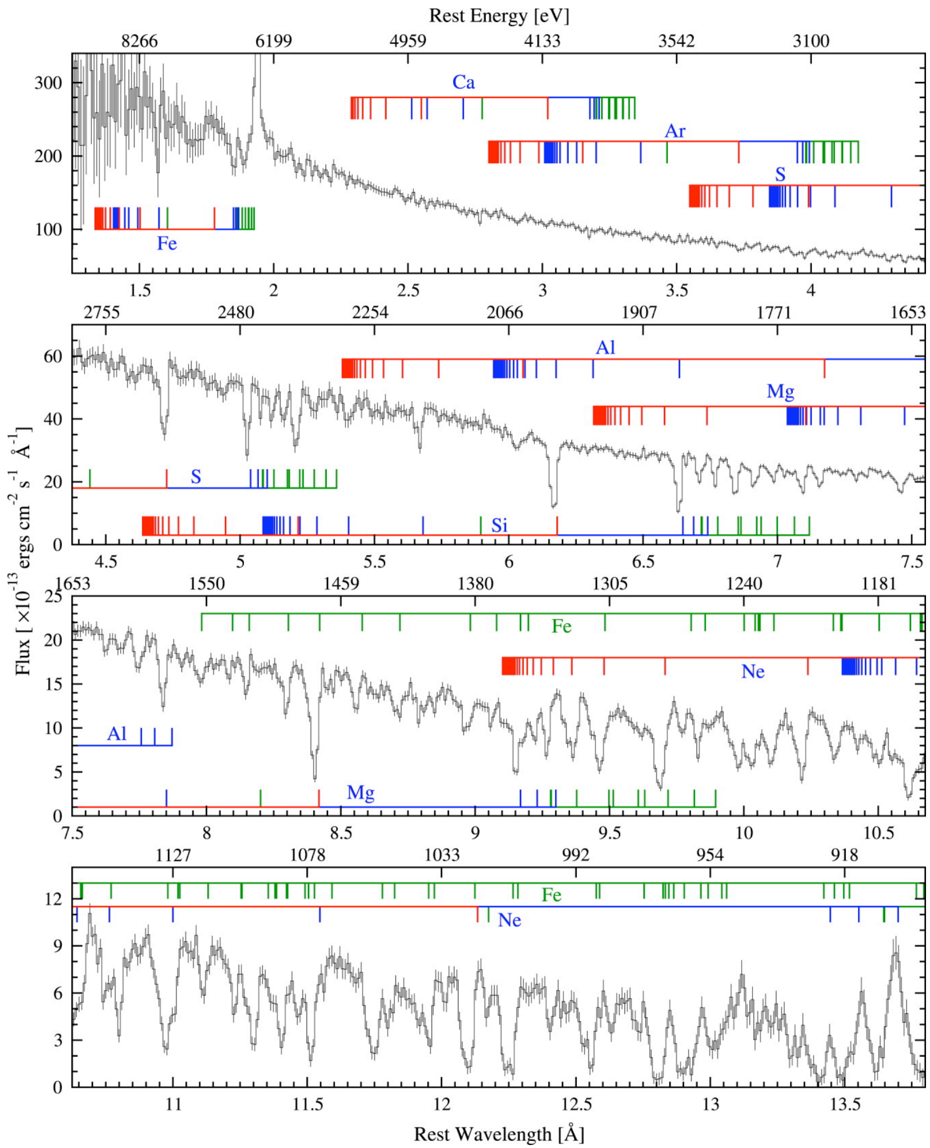


X-rays Sensitive to log ξ: -4 to 4 !!!

Seyfert 2 NGC 1068 : XMM RGS
Kinkhabwala et al. 2002



Seyfert 1 NGC 3783 : Chandra HETGS
Kaspi et al. 2000, 2002

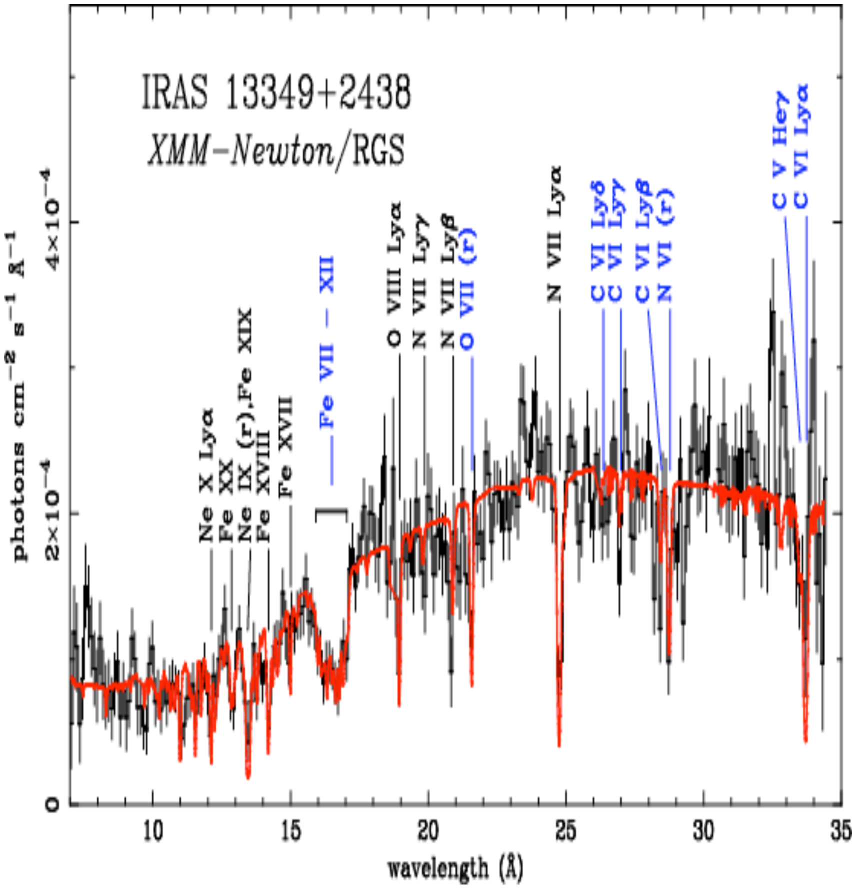


- See also Ogle et al. 2003 (Chandra HETGS) and Brinkman et al. 2002 (Chandra LETGS)

The Fe UTA (Fe0+ to Fe15+)

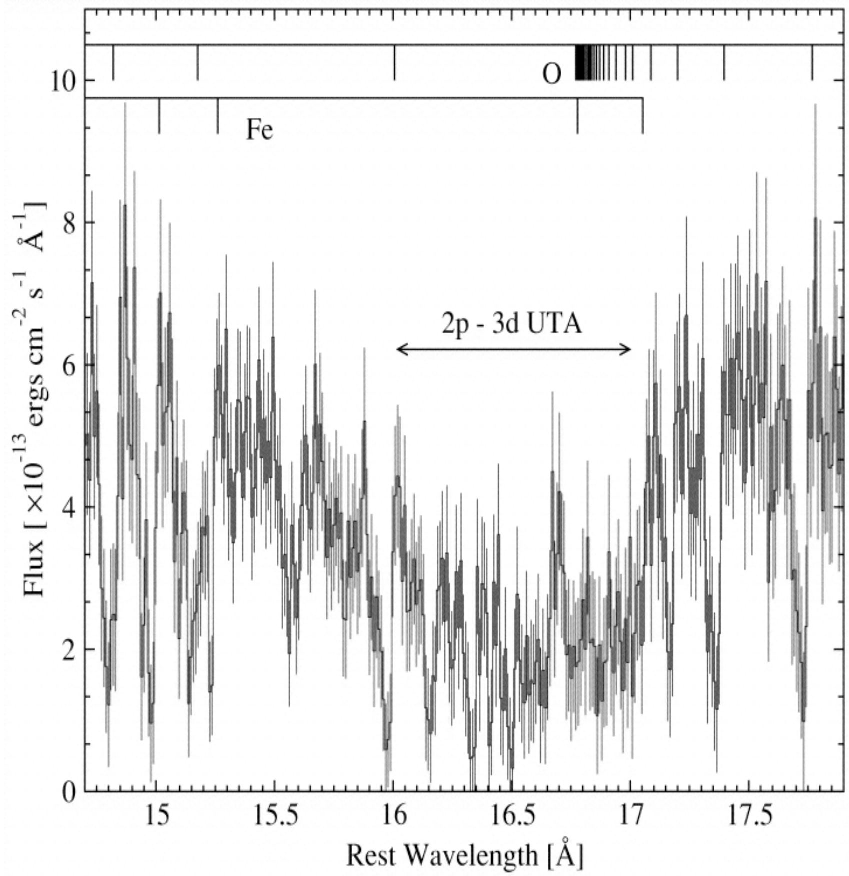
2p-3d transitions of M-shell Fe

XMM RGS : IRAS 13349+2438



Sako et al. 2001 A&A 365, L168

Chandra HETGS : NGC 3783



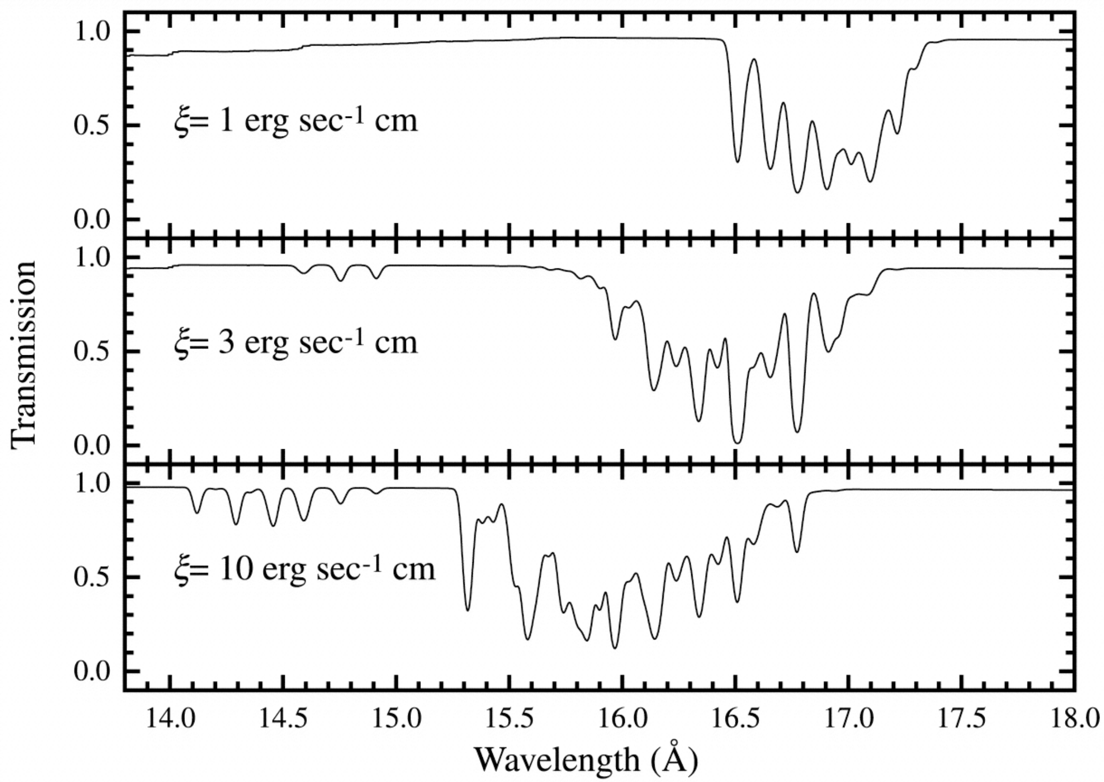
Kaspi et al. 2002, ApJ. 574, 643

For calculations : Behar, Sako, Kahn 2001; & Flexible Atomic Code (FAC) : Gu 2003

Absorption

Unresolved Transition Arrays (UTAs)

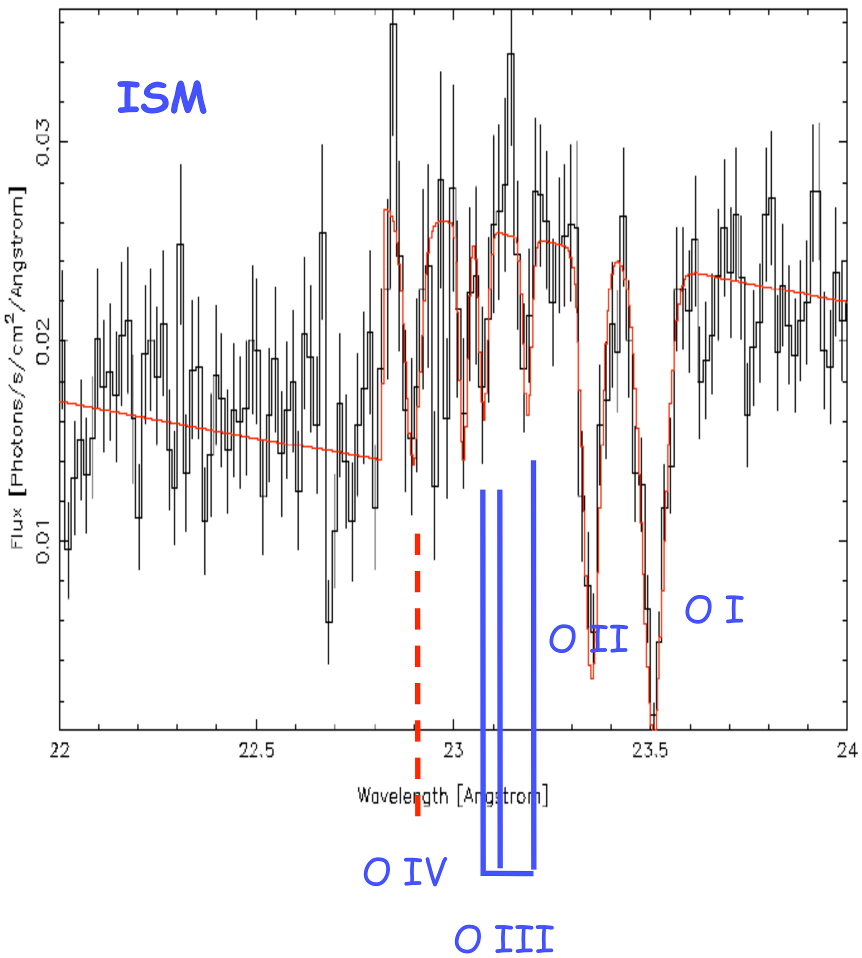
- Appears in absorption spectra of AGN, eg. NGC 3783
- Comes from 2p-3s or 2p-3d transitions --> requires iron less than 9 times ionized
- Potential diagnostic of ionization balance



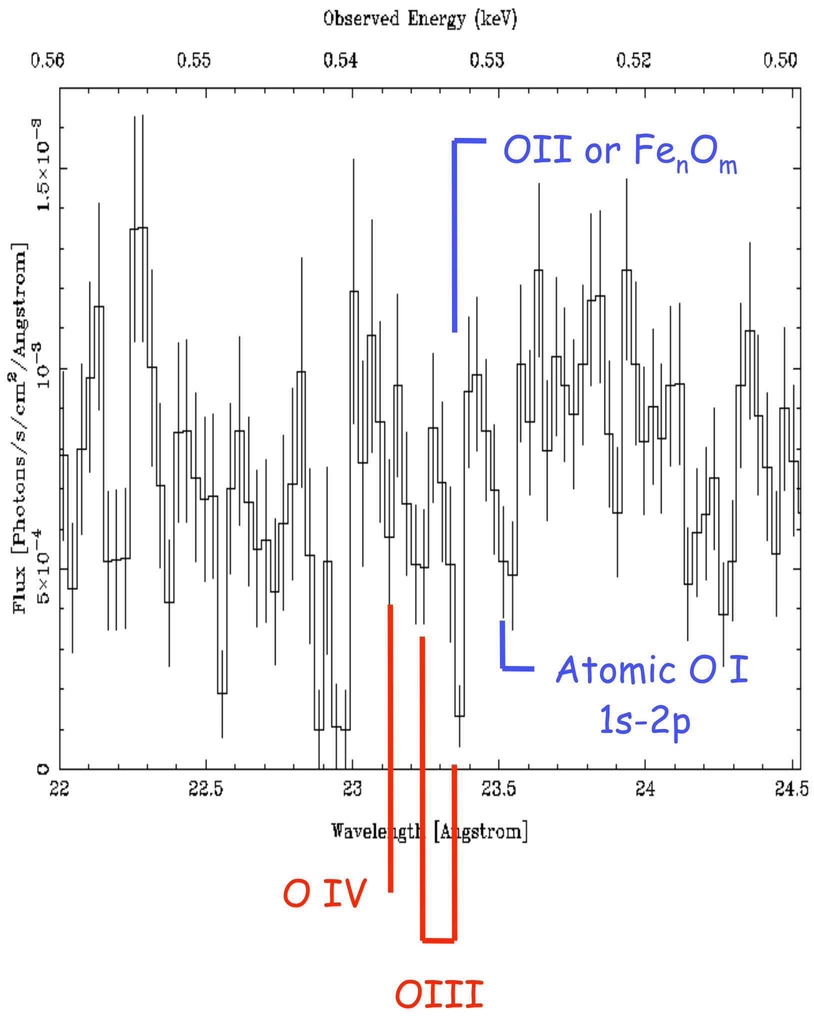
(Behar, Sako and Kahn 2002)

Innershell OI - OV

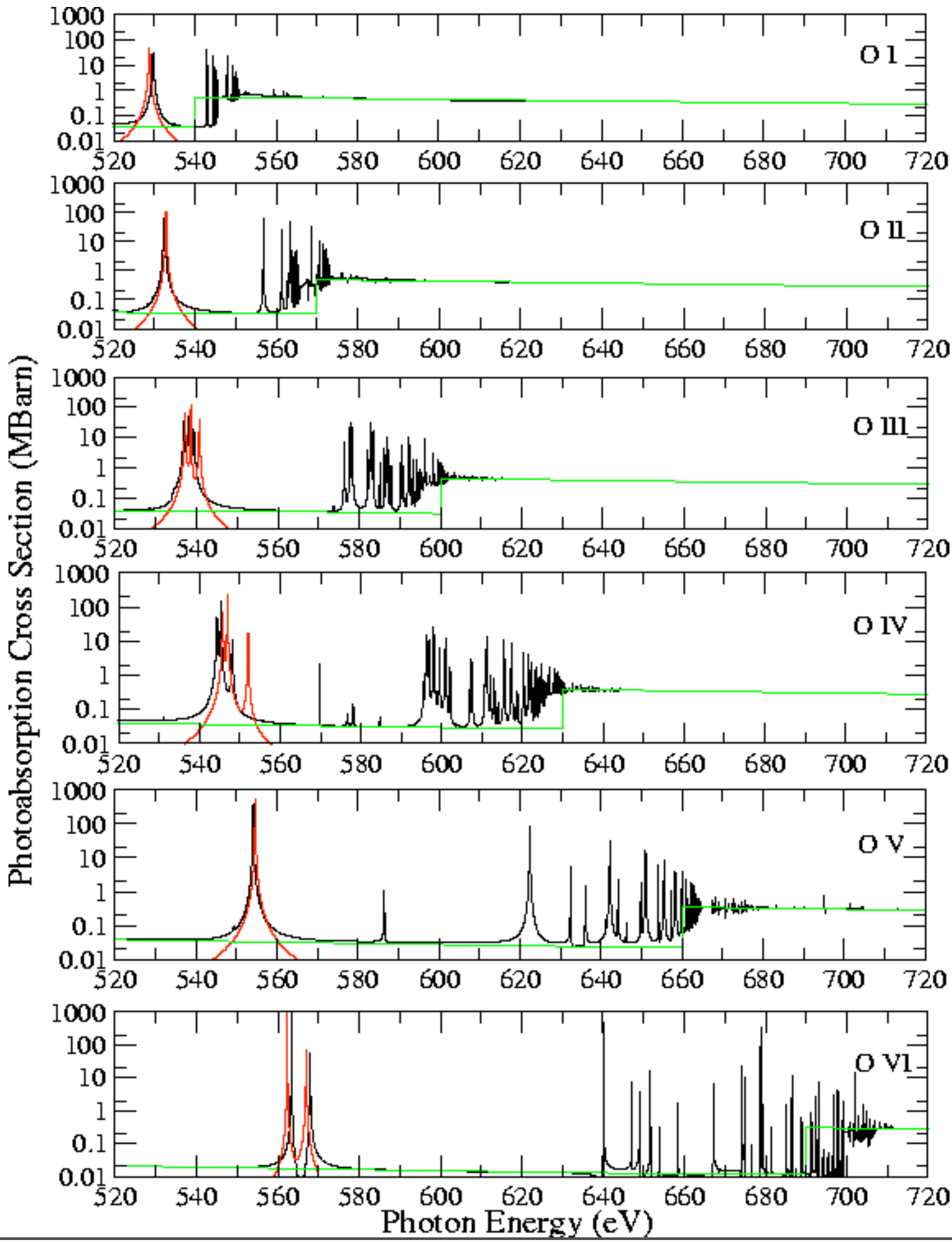
X-ray Binary : Juett et al.,2004



AGN : Lee et al. 2001



K shell Photoabsorption (Oxygen)

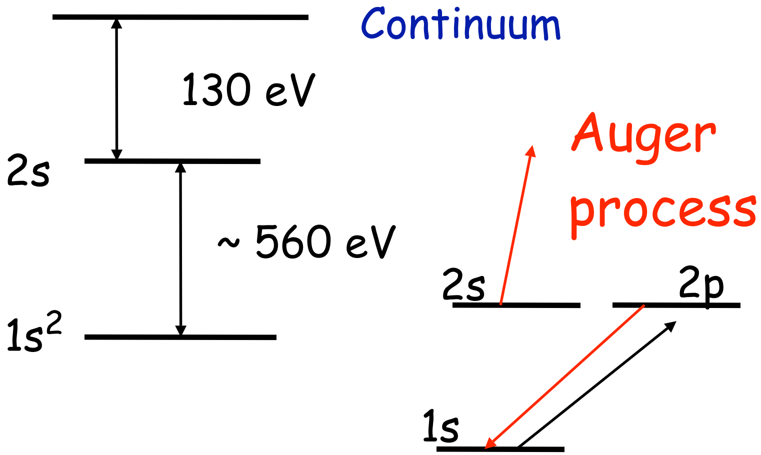


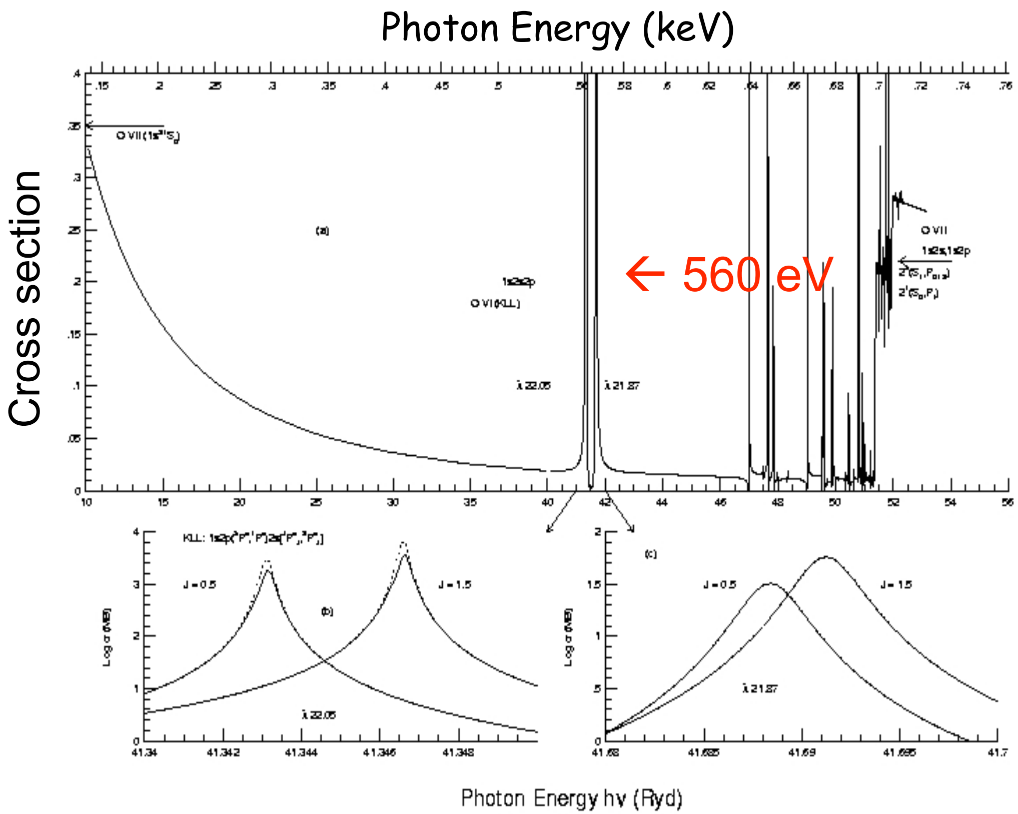
In theory, could diagnose ionization balance in the ISM or other absorbing material. This data uses semi-empirical corrections to energy levels in the optimization of wavefunctions, based on the experiment, plus multi-code approach

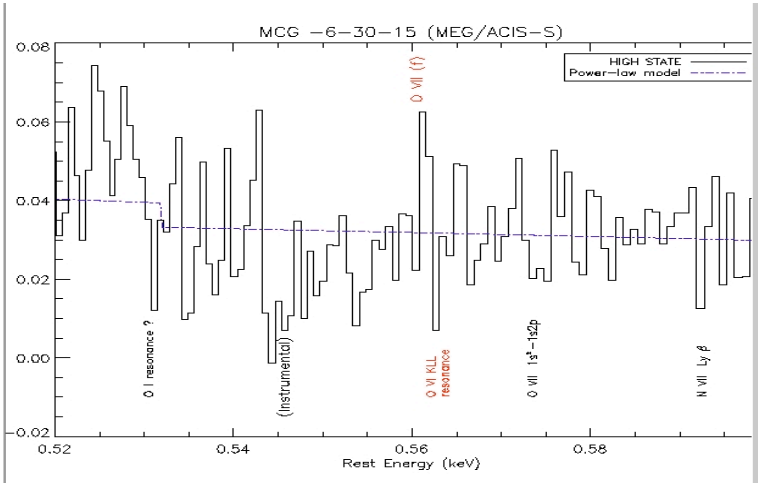
Red: Pradhan et al (2003)
Green: Verner and Yakovlev (1995)
Black: Garcia et al. (2005)

The KLL (1s2s2p) Resonance of O VI

Li-like O VI ($1s^2$ 2s)







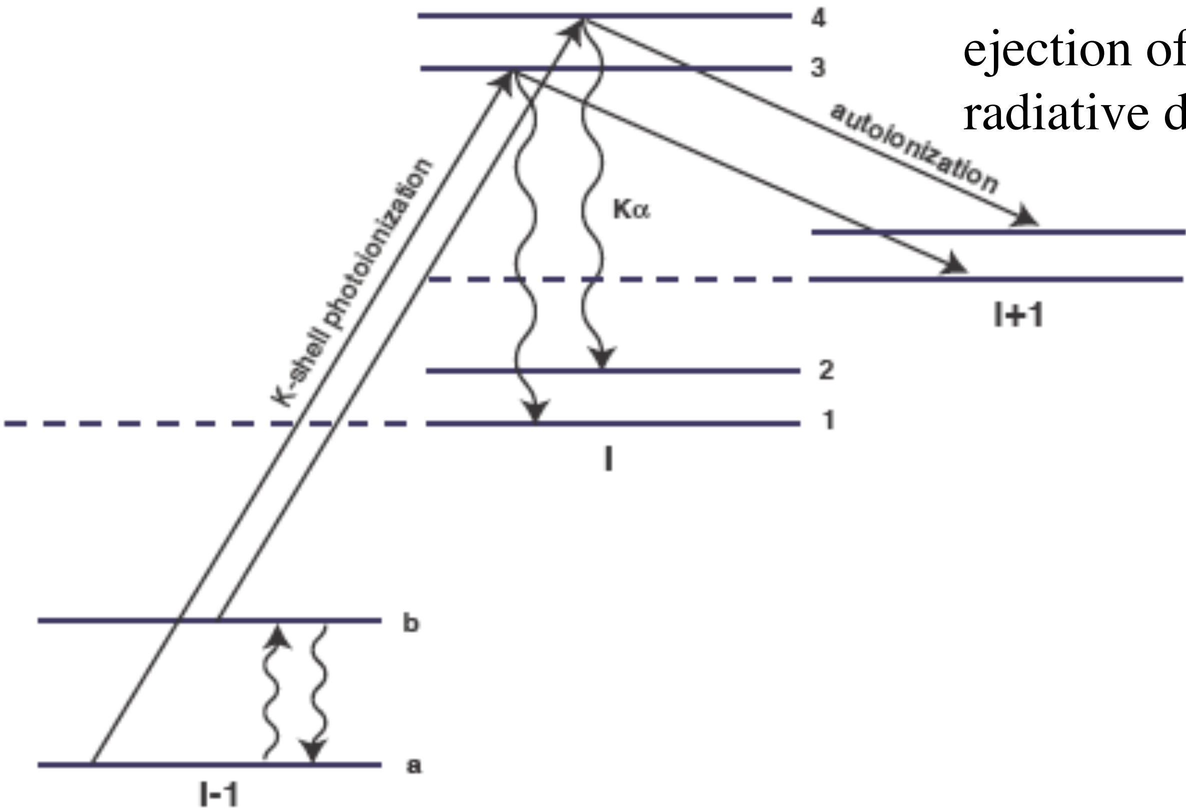
Pradhan 2000, *ApJ.*, 545, L165

←O VI in *MCG—6-30-15* (Lee et al. 2001)
N_{OVI} ~ 3 x 10^{17} cm^{-2}; EW ~ 32 mA

Also OV : Sako et al.,2003   O IV, Lee et al. 2003 in prep.

X-ray Fluorescence Lines from photoionized plasmas

Hard X-ray continuum in relatives cool ($T \sim 10^5$ - 10^6 K) matter



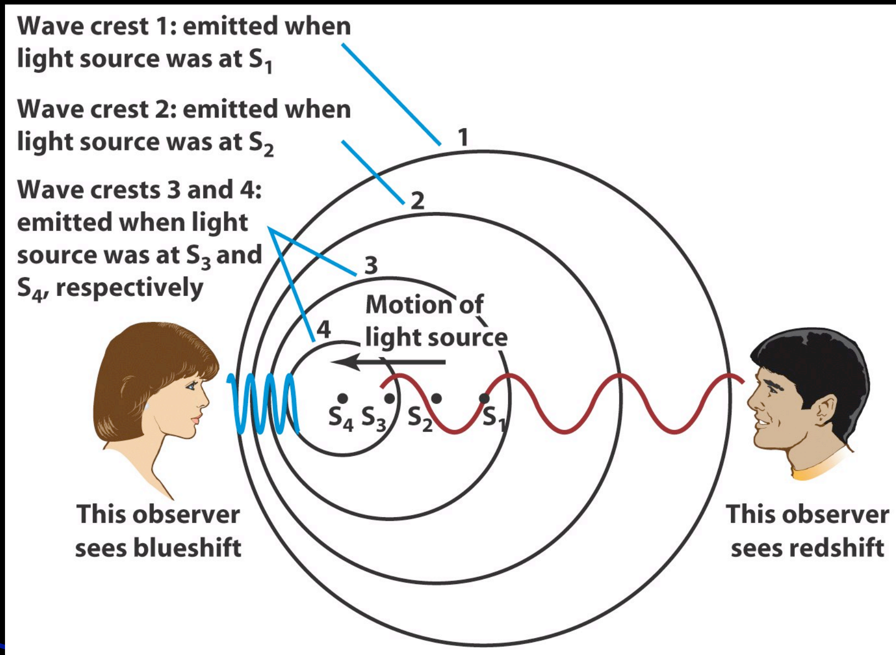
ejection of e- instead of radiative decay

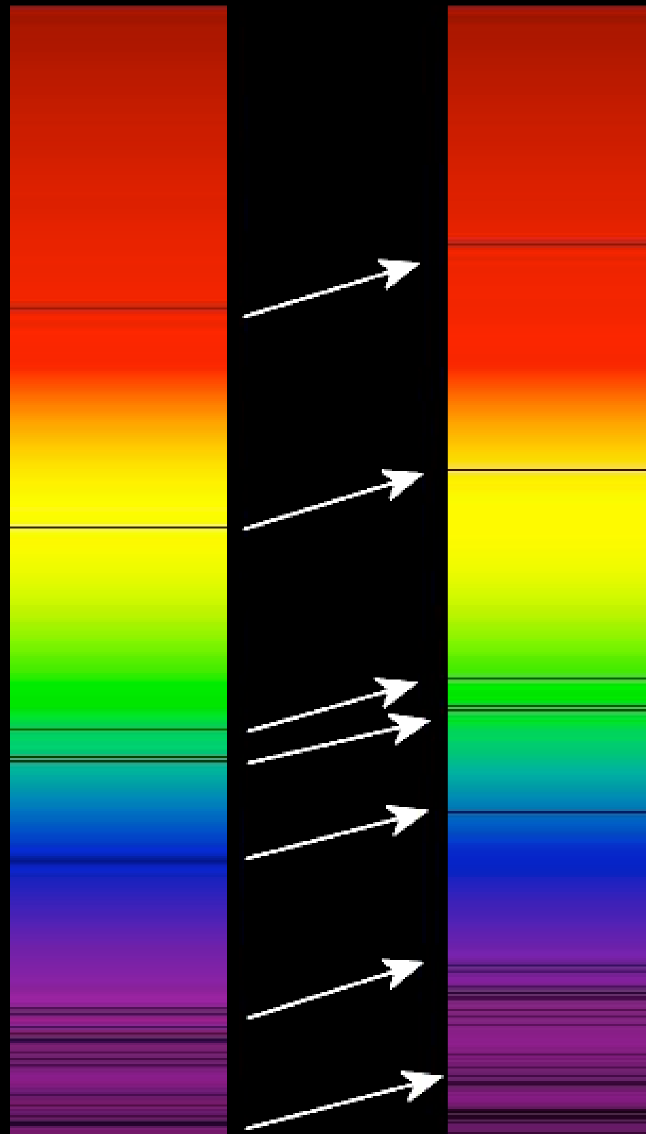
Diagram from Liedahl & Torres (2005)

There are lots of Physics in the lines

- Line position : ion identification
- **Line shifts: dynamics, e.g. inflow, outflow**
- Line strengths
  - ionic column : e.g. N_{OVII}, N_{NeX}, N_{FeXXVI} ...
  - degree of ionization : e.g. H-like/He-like
  - temperature, density
- Line widths : e.g. turbulence, GR

Dynamics : Inflow / Outflow Line (Doppler) Shifts





- This effect is detectable in the pattern of spectral lines!

- Shift given by:

$$\frac{\lambda - \lambda_0}{\lambda_0} \approx \frac{v \cos\theta}{c}$$

There are lots of Physics in the lines

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  - **degree of ionization : e.g. H-like, He-like**
  - **temperature, density**
- Line widths : e.g. turbulence, GR

Line strengths: absorption

Instructive example: transmission of continuum thru uniform slab

Optical depth

$$F_{\rm line} = F_{\rm cont}\exp(-\tau_\nu)$$

$$\tau_\nu = N_i\sigma_\nu = \frac{\pi e^2}{m_e c} f_{12}\, \phi_\nu; \quad \int \phi_\nu d\nu \equiv 1$$

Ion column density (cm^{-2})

Normalized profile

Oscillator strength (classically, f=1)

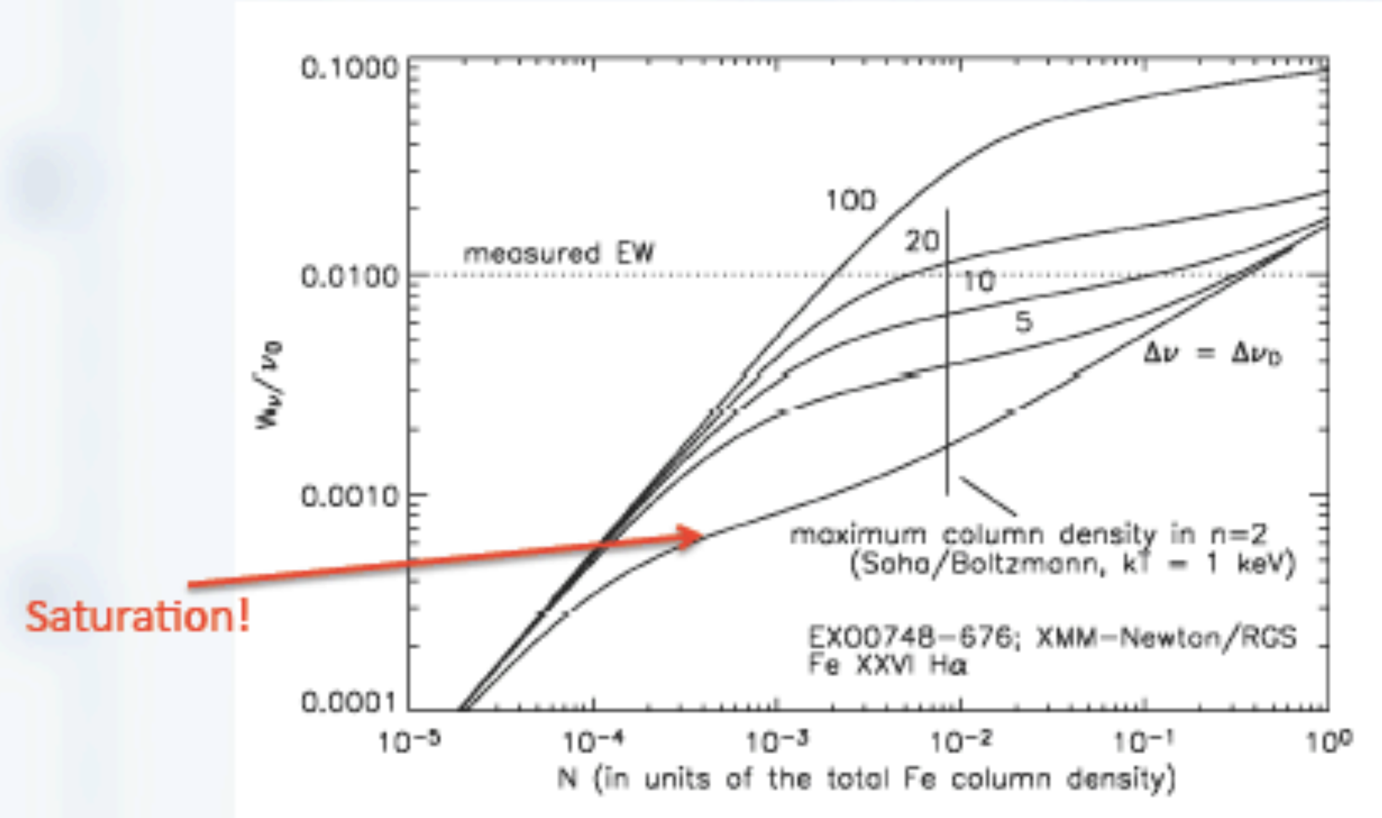
(cf. Rybicki and Lightman, Radiative Processes in Astrophysics)

Get this from classical damped harmonic oscillator!

Absorption/scattering cross section (cm^2)

Line strengths: absorption

EW as function of column density: 'curve of growth'



Analytic behavior easy to understand:

- $\tau_{\nu 0} << 1$: EW linear in N_i (all atoms absorb)
- $\tau_{\nu 0} \approx 1$: saturation; EW stalls at the Doppler width
- $\tau_{\nu 0} >> 1$: damping wings become optically thick; EW goes as $N_i^{1/2}$

Beware of saturation! If unresolved, lines look normal, but are in fact black

He-like Ions in Emission

Two electrons: can have |↑↑>, |↓↓>, |↑↓>, |↓↑>. But these are not all eigenstates of ***J***. These ones are:

|↑↑>, |↓↓>, |↑↓> + |↓↑> (symmetric in the spins, total spin 1) **'triplet'**

|↑↓> – |↓↑> (antisymmetric in the spins, total spin 0) | **'singlet'**

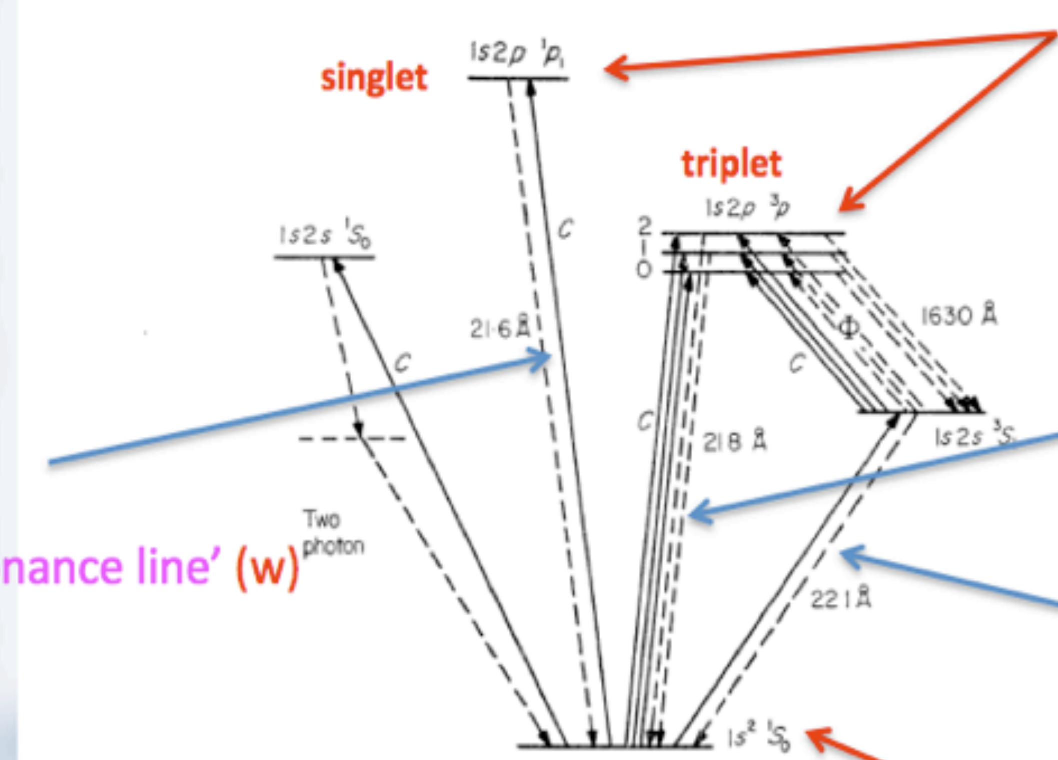


FIG. 1. *The He-like ion, showing those terms and processes involved in the present analysis. The wavelengths indicated apply to the case of oxygen* VII.

1s 2p; $L = l_1 + l_2 = 1$, so: P; four electron spin possibilities

'intercombination line(s)' (xy) (between triplet and singlet States; involves spin flip)

'resonance line' (w)

'forbidden line' (z) (LS forbidden)

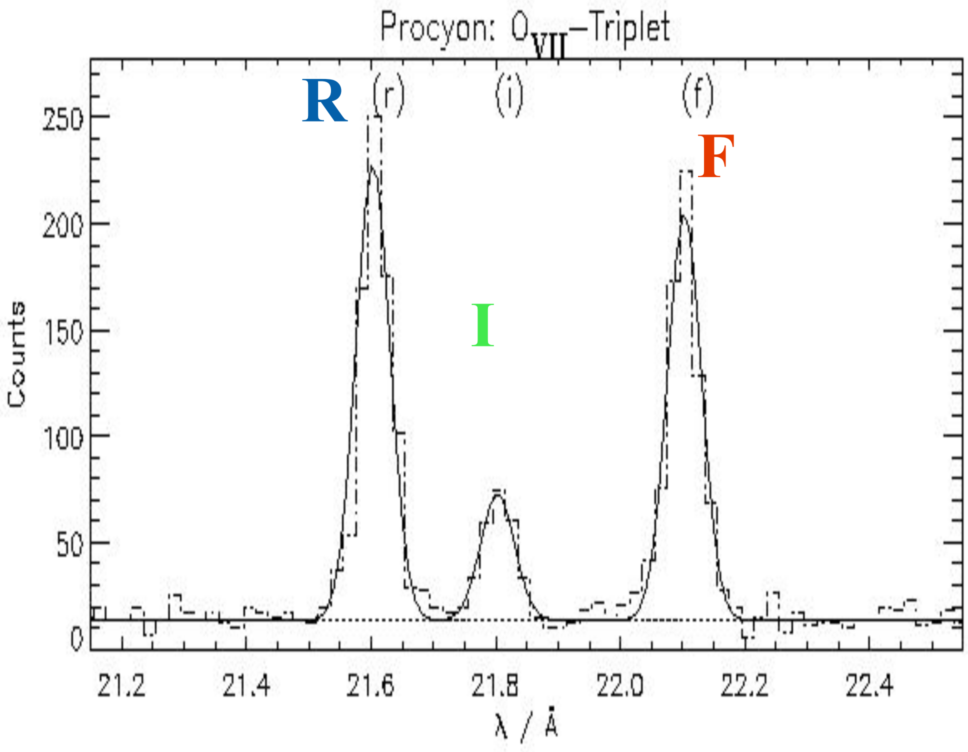
Ground: space-*symmetric*, must be spin-*antisymmetric*, so s = 0 (2s+1 = 1; **singlet**)

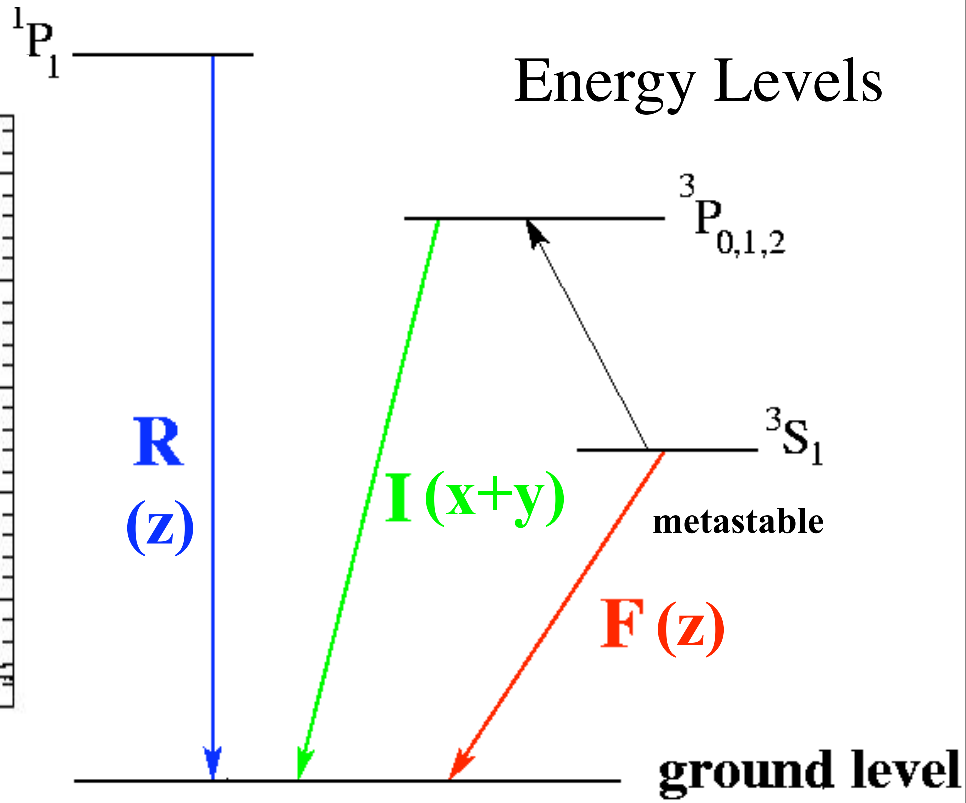
Gabriel and Jordan, 1969, *MNRAS*, **145**, 241

- Resonance (w) line
  - allowed electric dipole transitions involving ground state
- Intercombination (xy):
  - triplet (S=1) to singlet (S=0) state transition
    - S=0: no fine structure
    - S=1: 3 possible orientations of spin angular momentum
  - "spin forbidden"; usually seen for large Z, with large spin-orbit interaction; off-diagnoal matrix elements resulting in mixed eigenfunctions
- Forbidden (z)
  - a transition between 2 levels that is not allowed by selection rules for electric dipole radiation, i.e LS forbidden
  - metastable: states for which transitions from upper -> all lower levels are forbidden (transition through E transfer to other particle through collisions)
  - probability w-transitions rapidly increases with Z in hot plasmas
  - observed only when collisional de-excitation probability is low: e.g. astrophysical plasmas in solar corona & nebulae, and in some low density plasma in thermonuclear fusion devices

Plasma Diagnostics with He-like ions

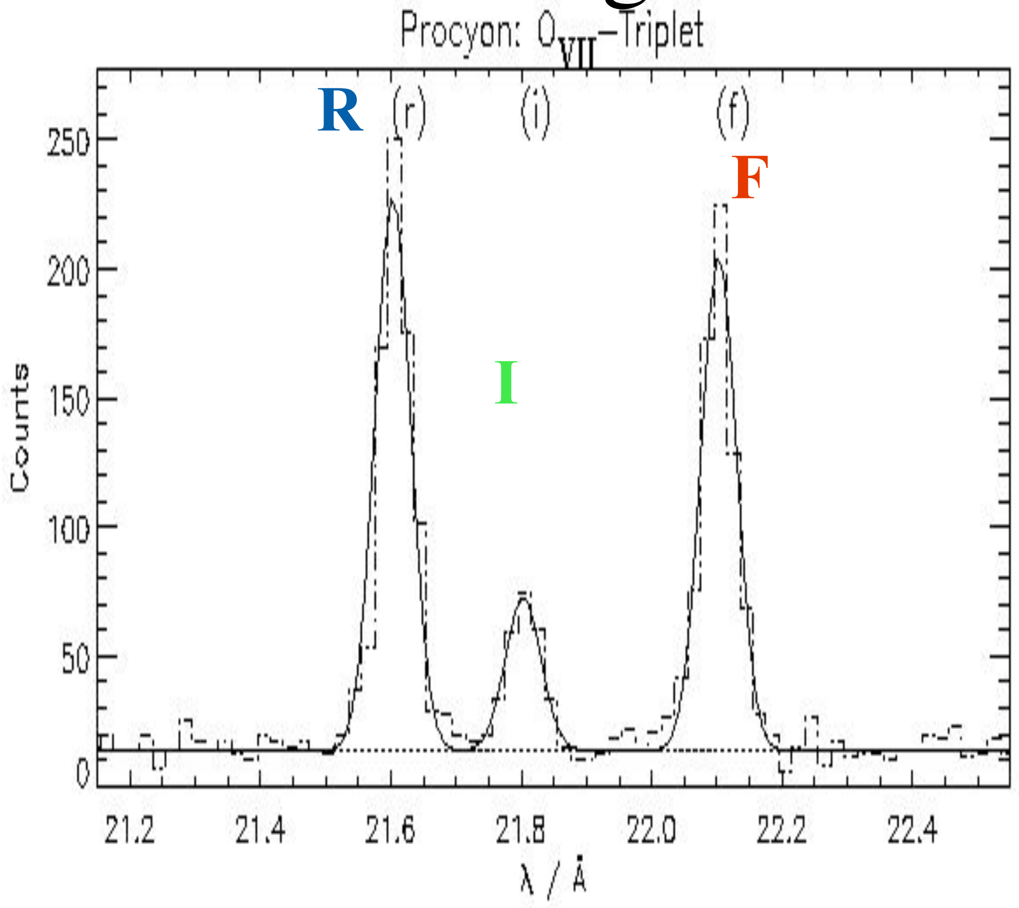
Density and Temperature Diagnostics





- Initial Usages: solar (coronal) plasma diagnostics; now extra solar objects
- Present Day: extra-solar objects:
  - Collisional (e.g., stellar coronae),
  - Photo-ionization (e.g., AGN, X-ray binaries), out-of-equilibrium (e.g., SNR)

Plasma Diagnostics with He-like ions



See papers by:

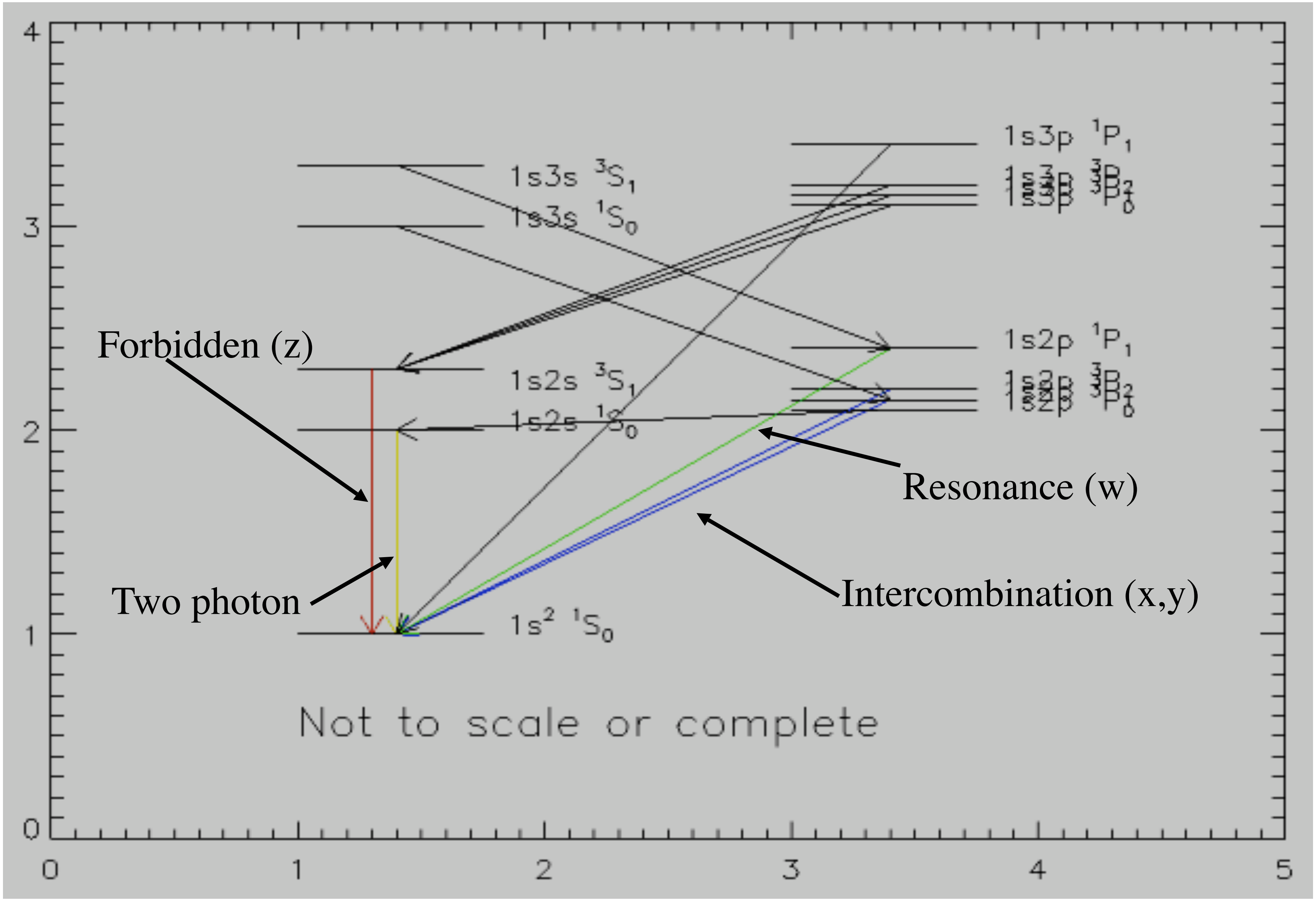
Pradhan (1985 -)
Liedahl (1999 -)
Mewe (1999 -)
Paerels (1998 -)

Gabriel & Jordan (1969): He-like Diagnostics

Density: $R(n_e)$ = **Forbidden** / **Intercombination** = **z** / **(x+y)**

Temperature: $G(T_e)$ = **(F + I)** / **Resonance** = **z** + **(x+y)** / **w**

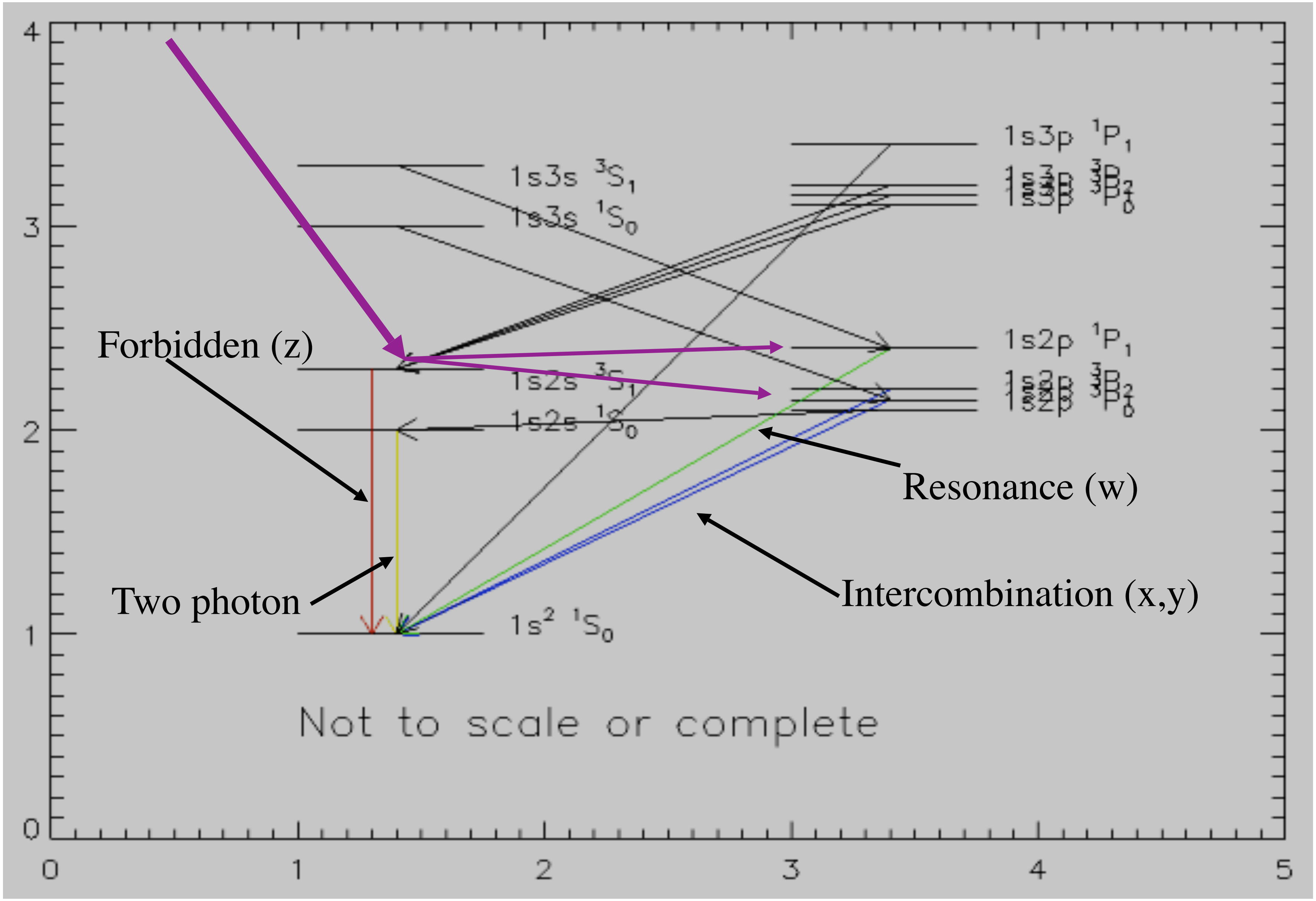
Density Diagnostics with R = F / I



Helium-like Lines

Density Diagnostics with R = F / I

If n_e is large enough, collisions move electrons from the forbidden to the intercombination and resonance levels.

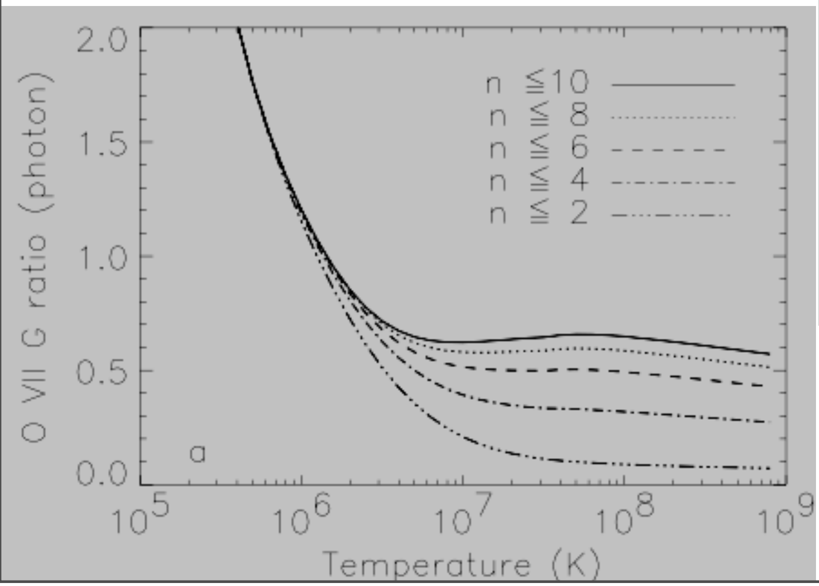


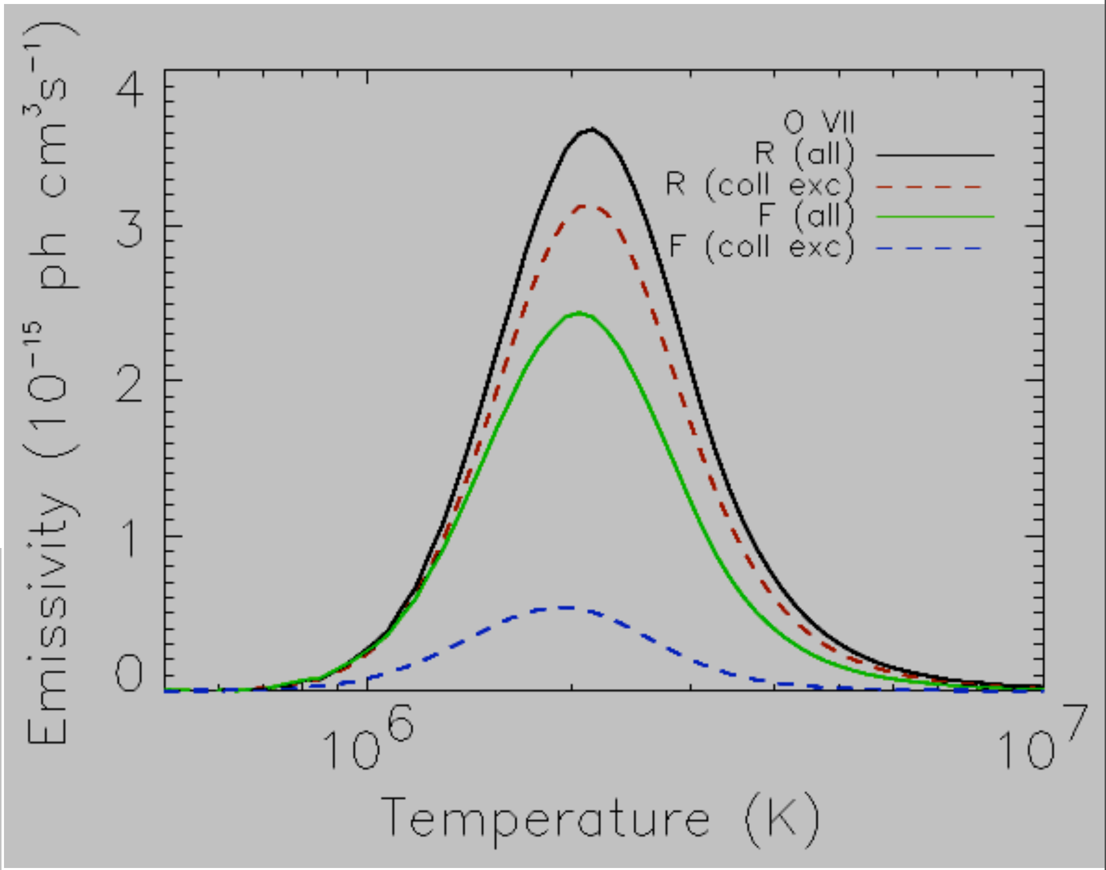
Helium-like Lines

Temperature Diagnostics with G=(F+I)/R

Why does the G ratio measure temperature and ionization state?

G = (F+I)/R



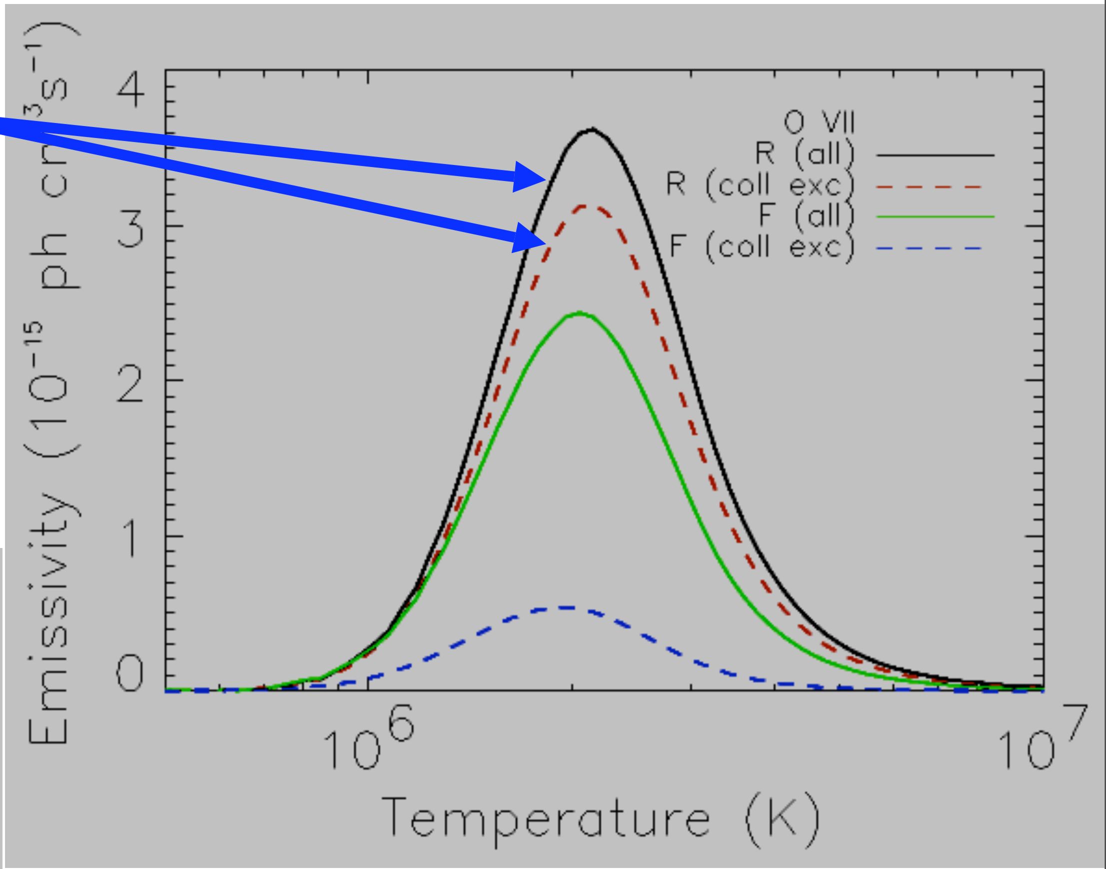


Helium-like Lines

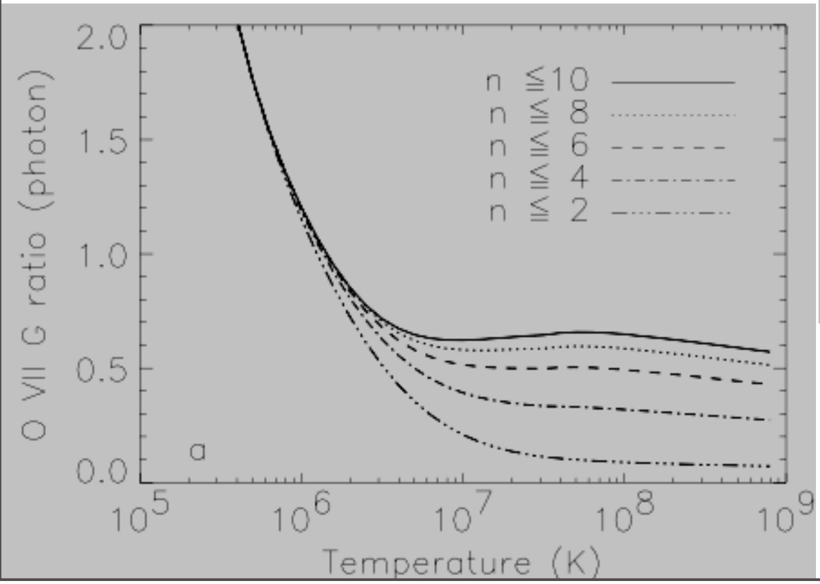
Temperature Diagnostics with G=(F+I)/R

Why does the G ratio measure temperature and ionization state?

Because the resonance line R is excited by collisions, which are temperature dependent,



G = (F+I)/R



Helium-like Lines

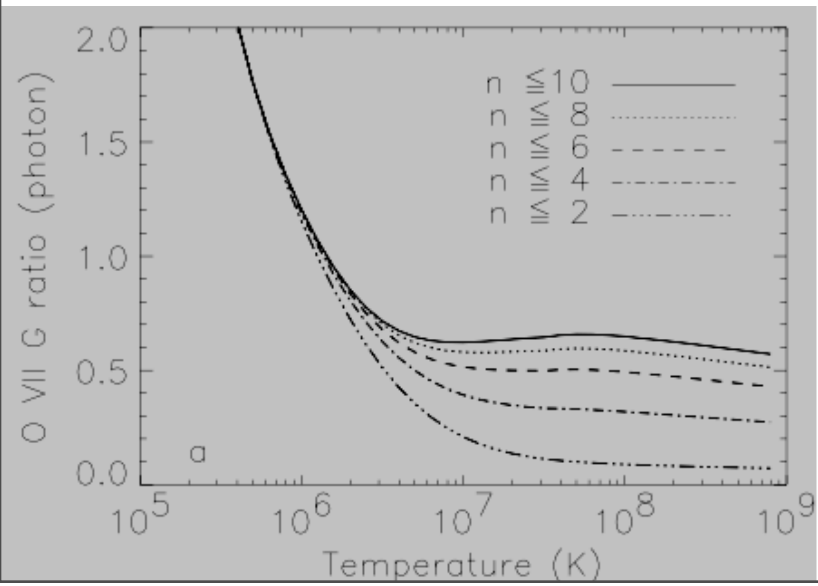
Temperature Diagnostics with G=(F+I)/R

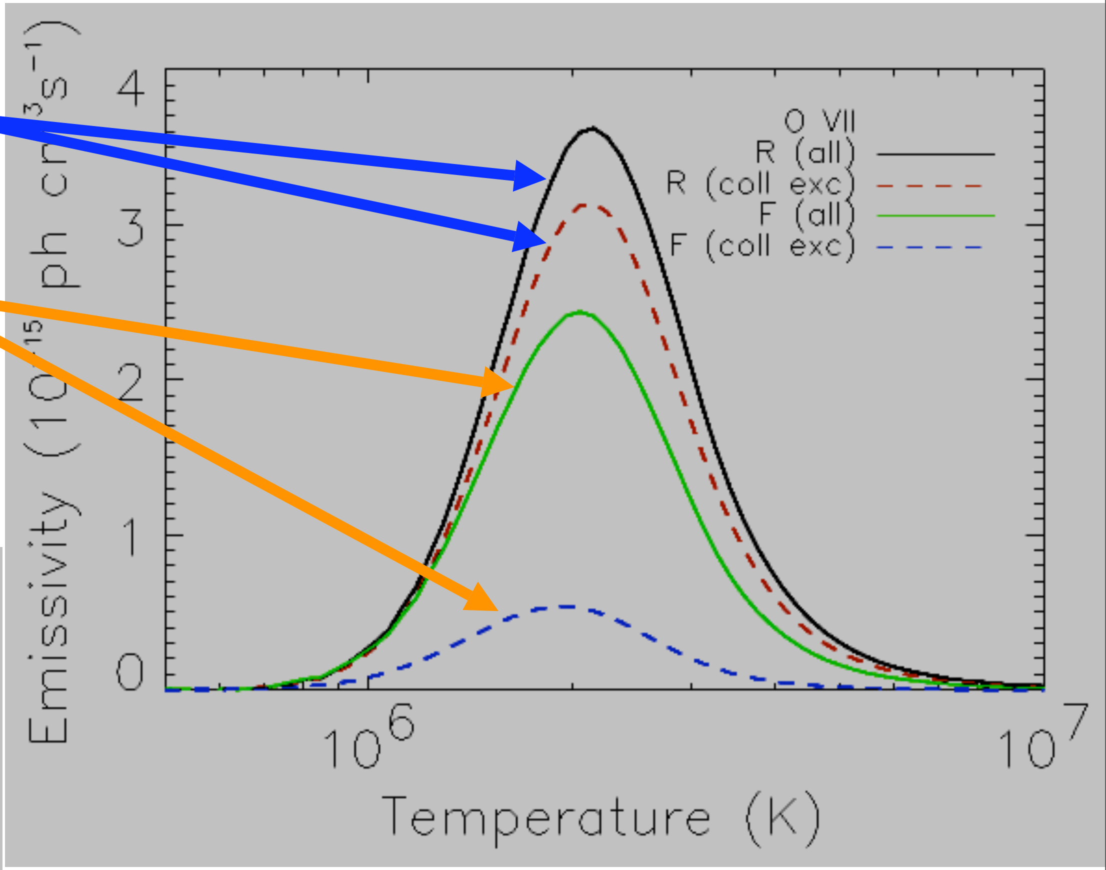
Why does the G ratio measure temperature and ionization state?

Because the resonance line R is excited by collisions, which are temperature dependent,

while the F and I lines are excited by recombination and other processes.

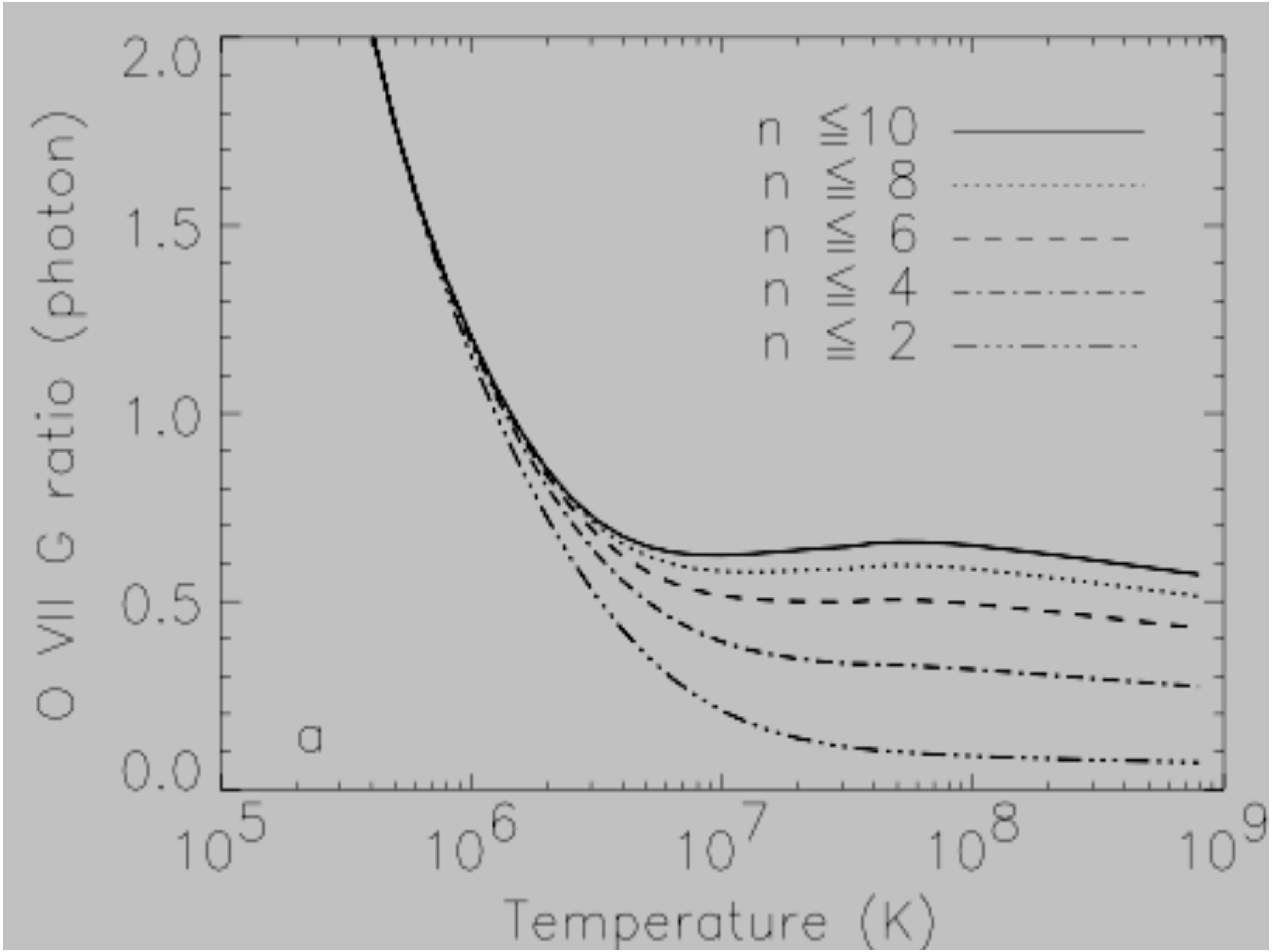
G = (F+I)/R





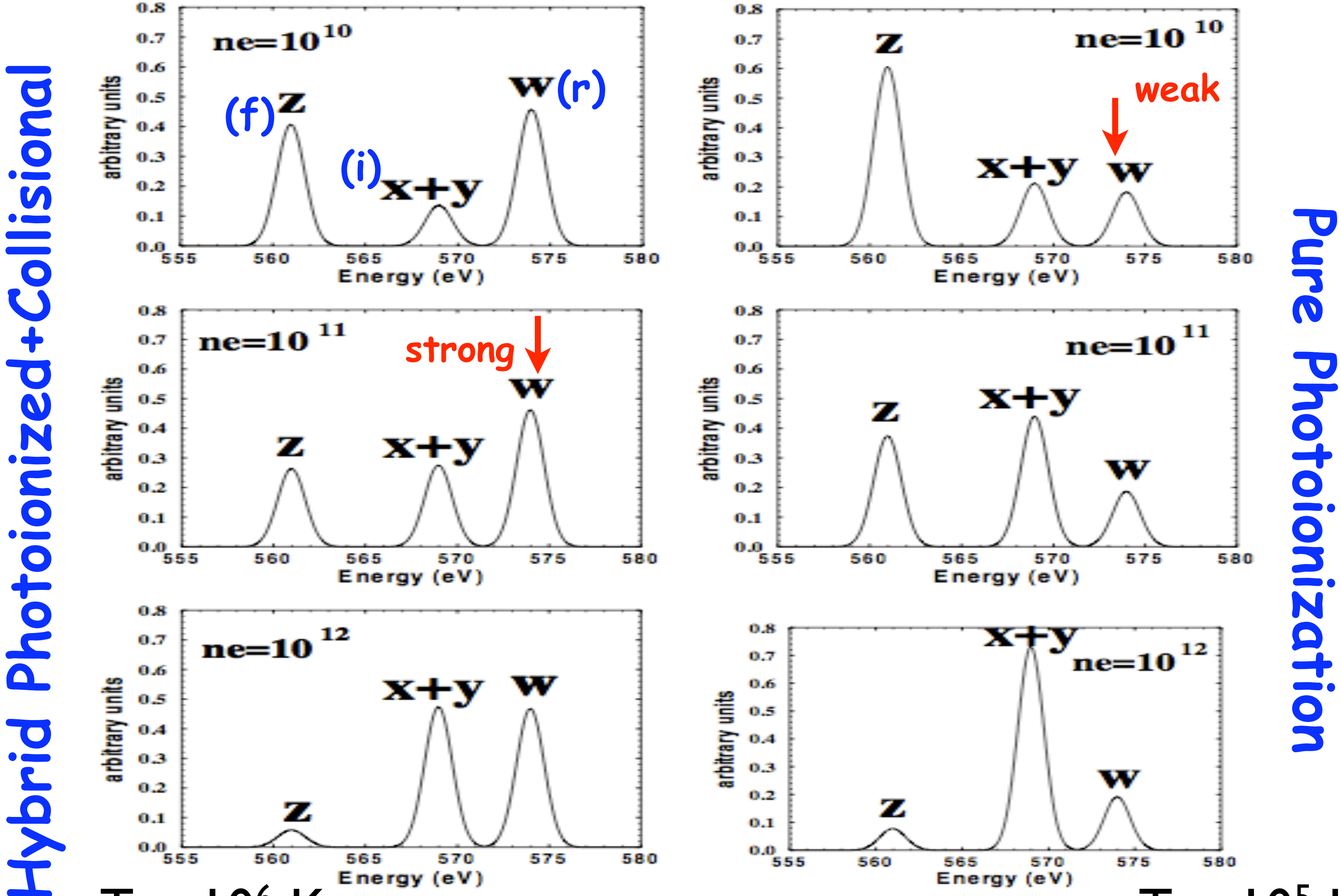
Helium-like Lines

Temperature Diagnostics with G=(F+I)/R



Helium-like Lines

Photoionized + Hybrid Plasmas for OVII

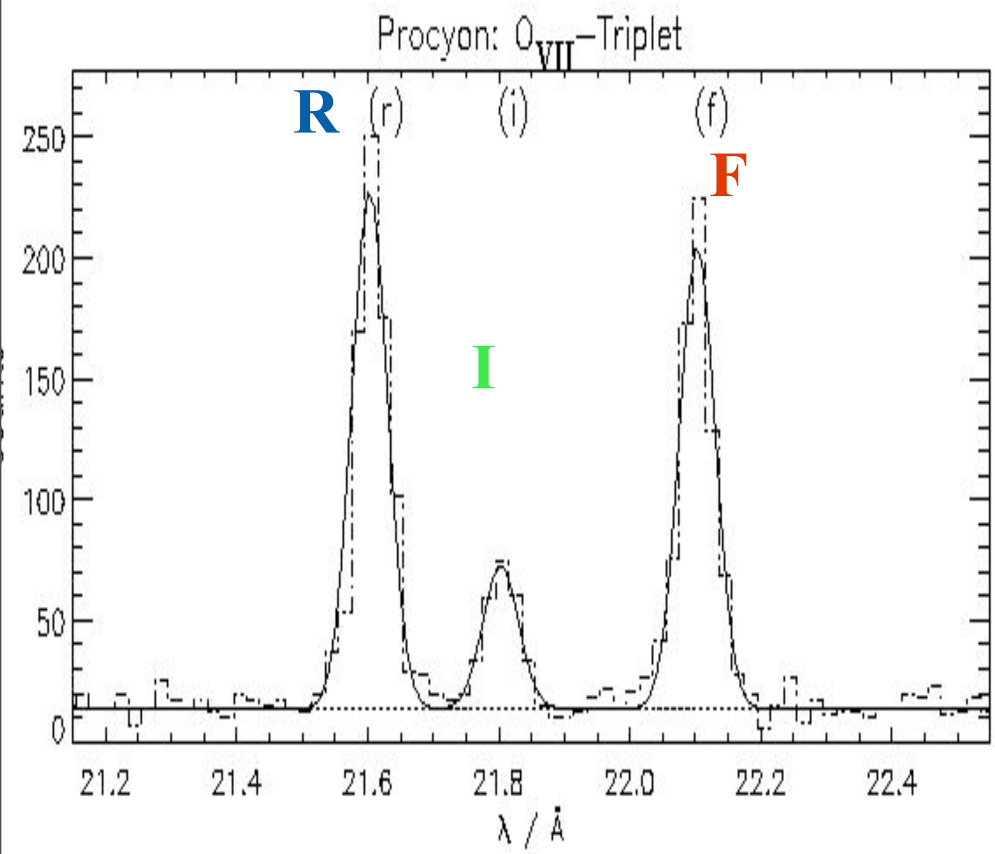


T = 10^6 K

T = 10^5 K

See Porquet & Dubau 2000, +

Plasma Diagnostics with He-like ions



Collisional Ionization: G~1

Photoionization/Hybrid: G > 1

Photoionization: G > 4

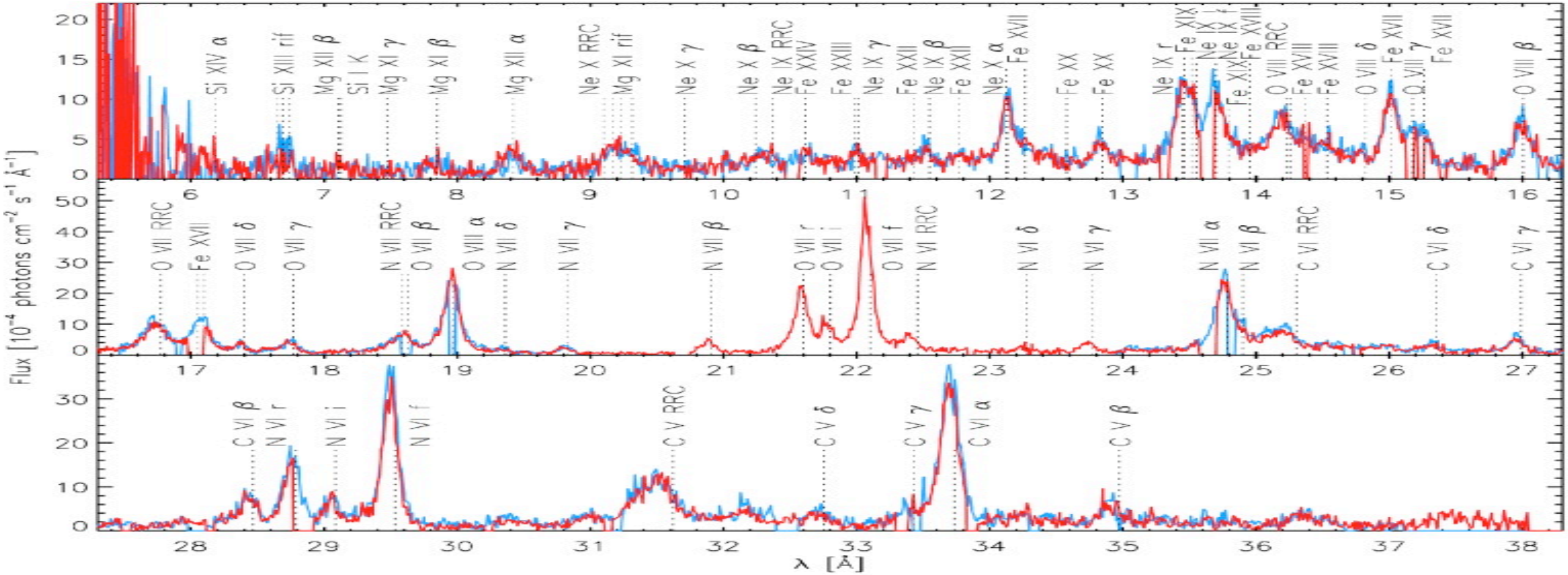
Gabriel & Jordan (1969): He-like Diagnostics

Density: $R(n_e)$ = **Forbidden** / **Intercombination** = **z** / (x+y)

Temperature: $G(T_e)$ = (**F** + **I**) / **Resonance** = **z** + (x+y) / **w**

Be Careful! He Triplet: Not a hard and fast rule ...

Seyfert 2 Galaxy NGC 1068:   Kinkhabwala et al. 2002; see also Ogle+ 03, Brinkman+ 03



- Photoexcitation ($n=1\rightarrow n_{i+1}$) can mimic the “signatures” of collisionally ionized plasma
  - misleading G since R gets enhanced through recombination
- Solution:
  - Look @ higher order lines
    - photoexcitation will enhance high order lines more than allowed in CI plasma
  - Look for RRC
    - CI plasma: RRC smeared out: E(captured e^-) < E(ion) so do not contribute much more E to atom
    - PI plasma: DV gives T: E(captured e^-) >> E(ion) so contribute a lot more E

Line strengths: absorption

Instructive example: transmission of continuum thru uniform slab

Optical depth

$$F_{\rm line} = F_{\rm cont} \exp(-\tau_\nu)$$

$$\tau_\nu = N_i \sigma_\nu = \frac{\pi e^2}{m_e c} f_{12}\, \phi_\nu; \quad \int \phi_\nu d\nu \equiv 1$$

Normalized profile

Ion column density (cm^{-2})

Oscillator strength (classically, f=1)

(cf. Rybicki and Lightman, Radiative Processes in Astrophysics)

Get this from classical damped harmonic oscillator!

Absorption/scattering cross section (cm^2)

Line strengths: absorption

General profile: convolution of Lorentzian with Gaussian: ***Voigt***
Parameter: ratio of damping width to Doppler width

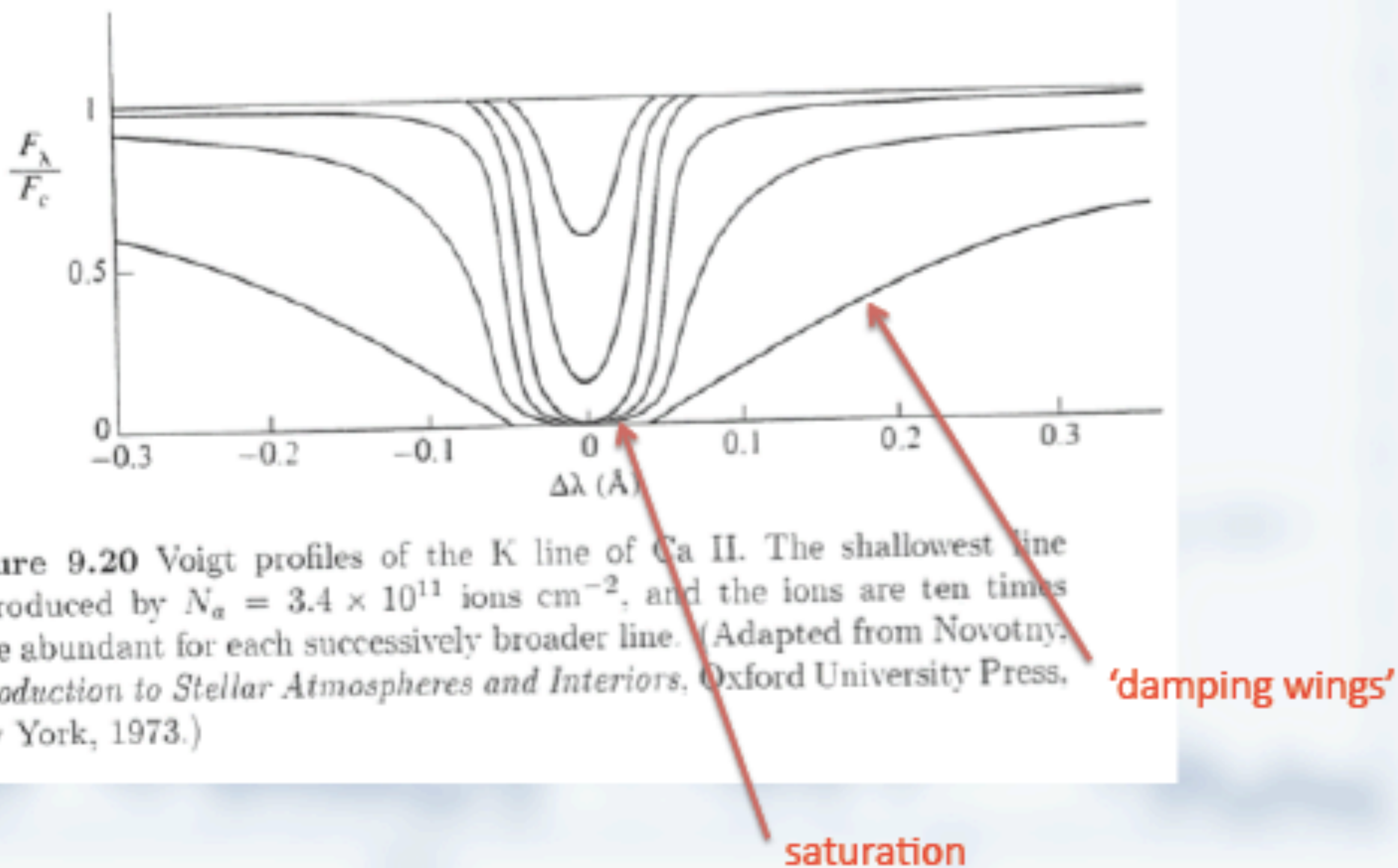


Figure 9.20 Voigt profiles of the K line of Ca II. The shallowest line is produced by $N_a = 3.4 \times 10^{11}$ ions cm^{-2}, and the ions are ten times more abundant for each successively broader line. (Adapted from Novotny, *Introduction to Stellar Atmospheres and Interiors*, Oxford University Press, New York, 1973.)

From Carroll and Ostlie: Introduction to Modern Astrophysics

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- Line position : ion identification
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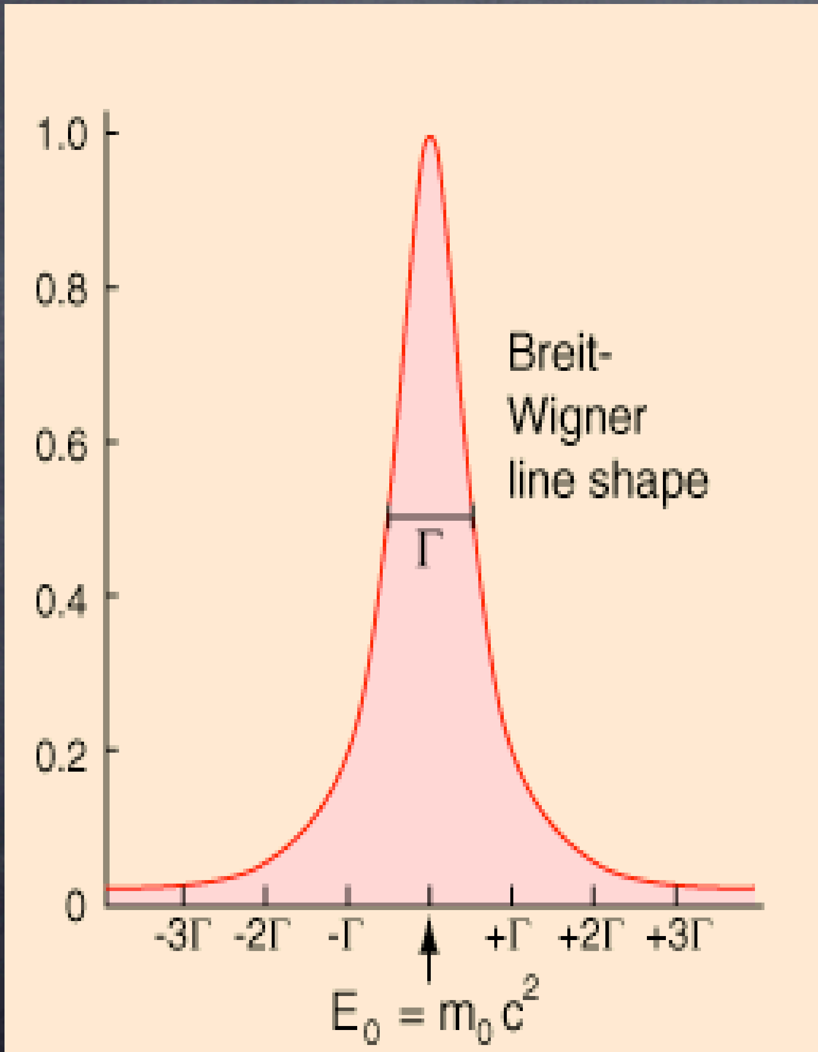
  - temperature, density
- **Line widths : e.g. turbulence, GR**

Natural Broadening

Due to finite lifetime of ionic/excited states



- Arises from the uncertainty in energy of the states involved in the transition
  - Heisengberg's Uncertainty Principle
- Not important in atomic spectra since lifetime of atomic transitions are $T \sim 10^{-8}$ s
  --> Natural LW ~ 6.6×10^{-8} eV

Single ion: Lorentzian, with characteristic width given by the lifetime of the upper level involved in the transition ('natural broadening', or 'damping')

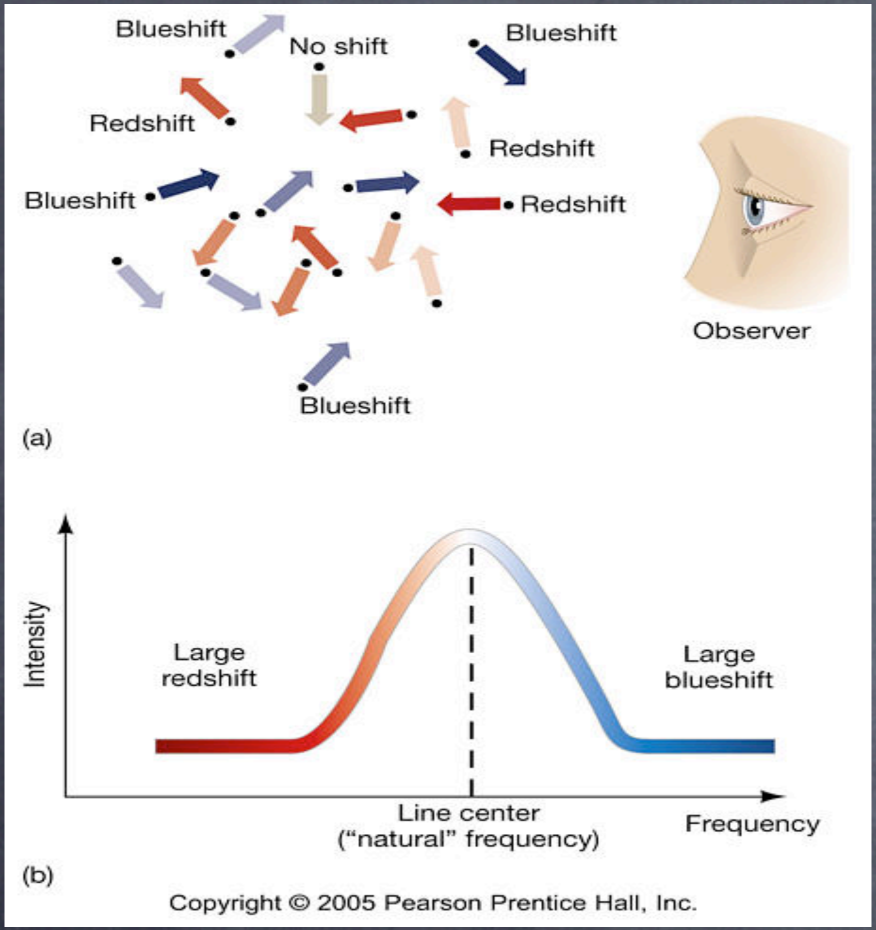
$$\phi_\nu = \frac{\Gamma/4\pi^2}{(\nu-\nu_0)^2 + (\Gamma/4\pi)^2}$$

and any other process that limits the lifetime (e.g. collisions)

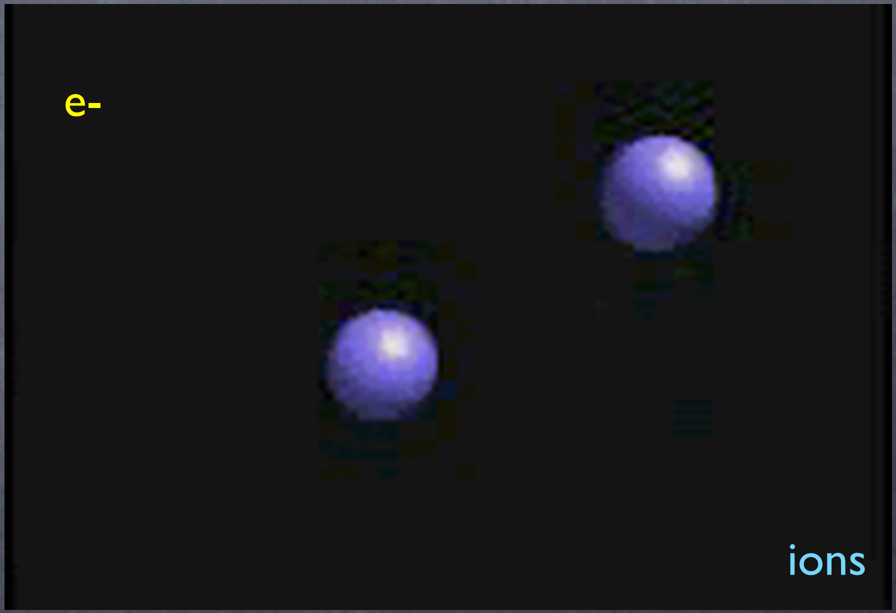
Thermal & Turbulent Broadening

Thermal Broadening: Atoms in constant thermal motion in cloud of gas, which "smear" line in Gaussian profile

Thermal & Turbulent Broadening

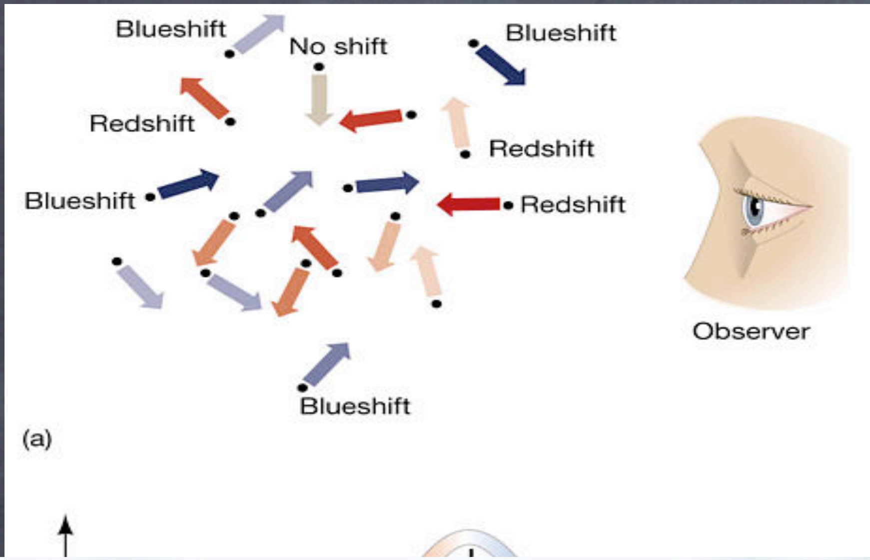


Turbulent Broadening: Exists when a cloud is not at rest / flowing smoothly, but churning in eddies and vortices: motion cause (random) Doppler shifting of spectral lines from different parts of cloud that cannot be discerned by telescope

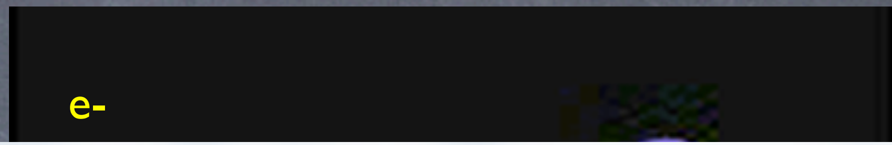


Thermal Broadening: Atoms in constant thermal motion in cloud of gas, which "smear" line in Gaussian profile

Thermal & Turbulent Broadening



Turbulent Broadening: Exists when a cloud is not at rest / flowing smoothly, but churning in eddies and vortices: motion cause (random) Doppler shifting of spectral lines from different parts of cloud that cannot be discerned by telescope



Broadening by radial velocities of ions, e.g. thermal velocities: Gaussian profile

$$\phi_\nu = \frac{1}{\Delta\nu_D\sqrt{\pi}} \exp\left(-(\nu-\nu_0)^2/\Delta\nu_D^2\right)$$

$$\Delta\nu_D/\nu_0 = \left(\frac{2kT}{m_i c^2}\right)^{1/2}$$

and any other process that produces a velocity broadening (e.g. turbulence)

Thermal Doppler width

Line strengths: absorption

Line profile:

Single ion: Lorentzian, with characteristic width given by the lifetime of the upper level involved in the transition ('natural broadening', or 'damping')

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

and any other process that limits the lifetime (e.g. collisions)

Broadening by radial velocities of ions, e.g. thermal velocities: Gaussian profile

$$\phi_\nu = \frac{1}{\Delta\nu_D\sqrt{\pi}} \exp\left(-(\nu - \nu_0)^2/\Delta\nu_D^2\right)$$

$$\Delta\nu_D/\nu_0 = \left(\frac{2kT}{m_i c^2}\right)^{1/2}$$

and any other process that produces a velocity broadening (e.g. turbulence)

Thermal Doppler width

How you model your lines will affect your flux and therefore determination of plasma column density.

Line strengths: absorption

General profile: convolution of Lorentzian with Gaussian: *Voigt*
Parameter: ratio of damping width to Doppler width

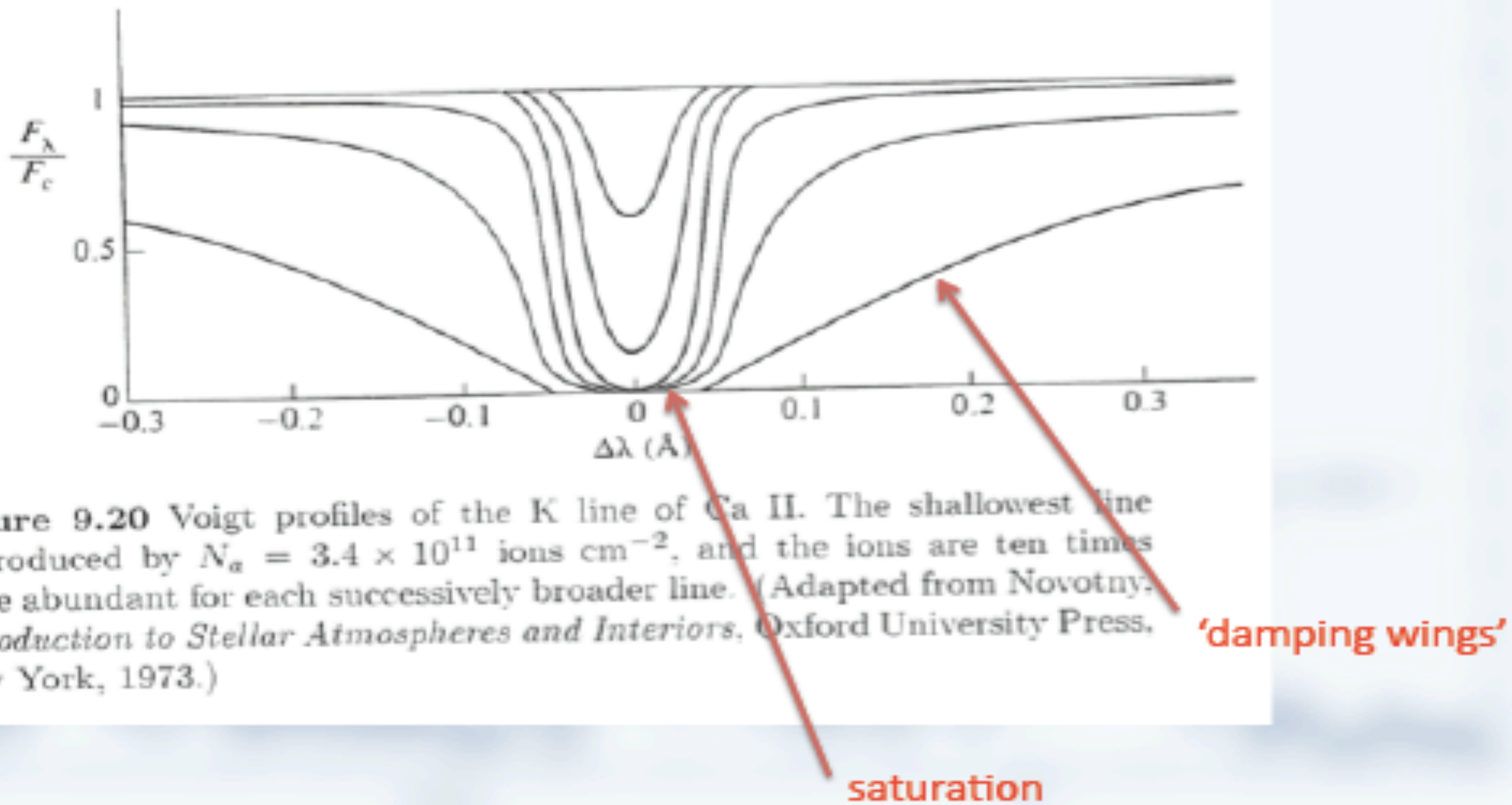


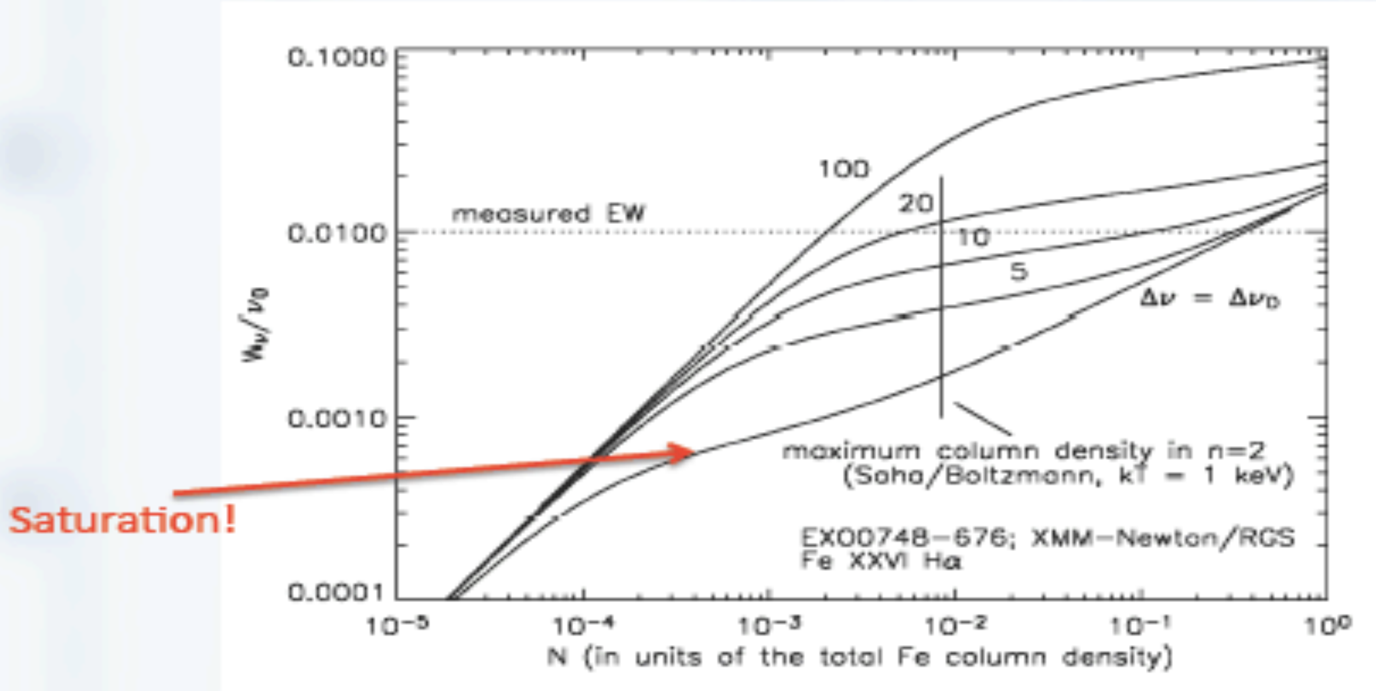
Figure 9.20 Voigt profiles of the K line of Ca II. The shallowest line is produced by $N_a = 3.4 \times 10^{11}$ ions cm^{-2}, and the ions are ten times more abundant for each successively broader line. (Adapted from Novotny, *Introduction to Stellar Atmospheres and Interiors*, Oxford University Press, New York, 1973.)

From Carroll and Ostlie: Introduction to Modern Astrophysics

How you model your lines will affect your flux and therefore determination of plasma column density.

Line strengths: absorption

EW as function of column density: 'curve of growth'

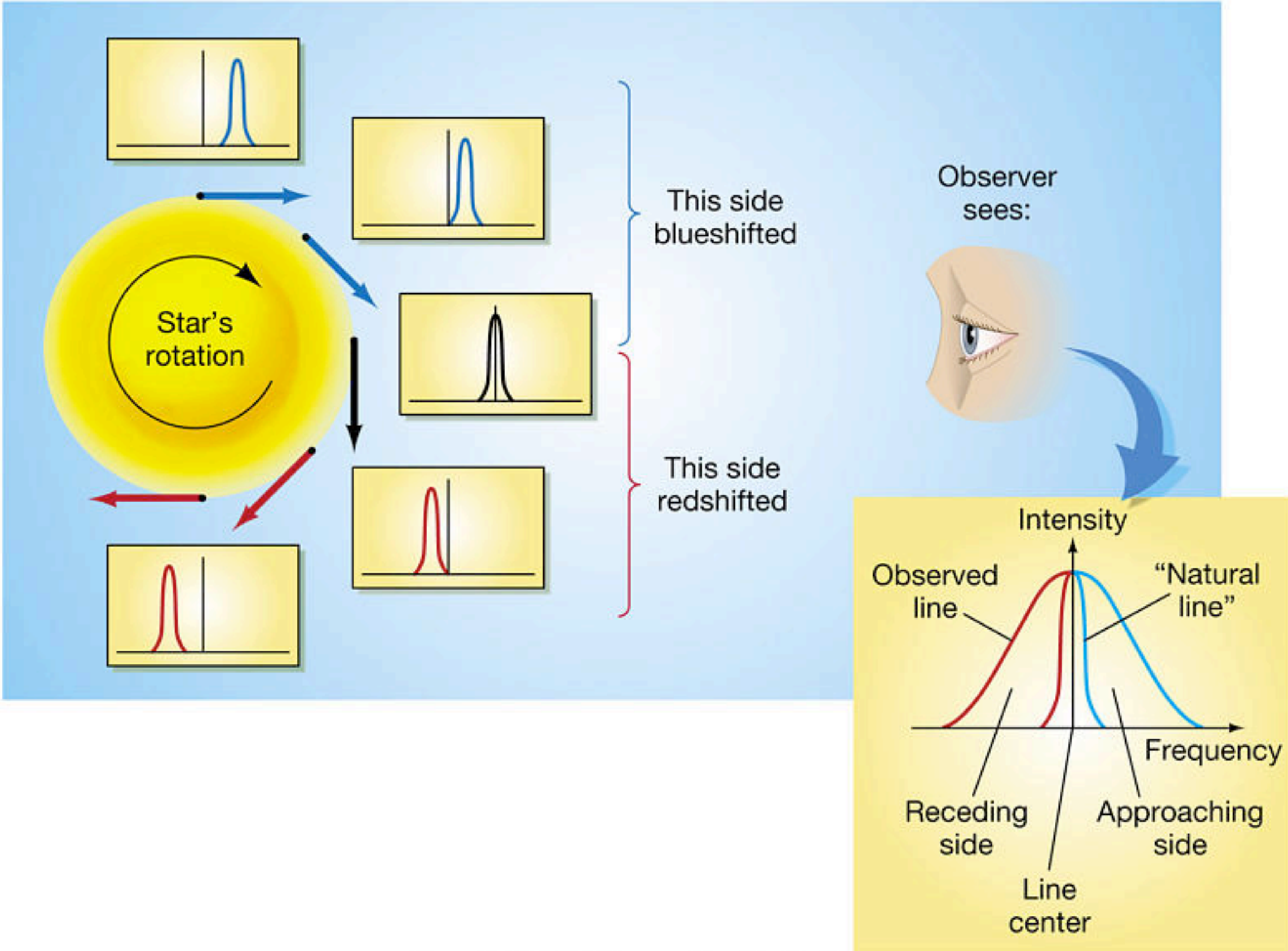


Analytic behavior easy to understand:

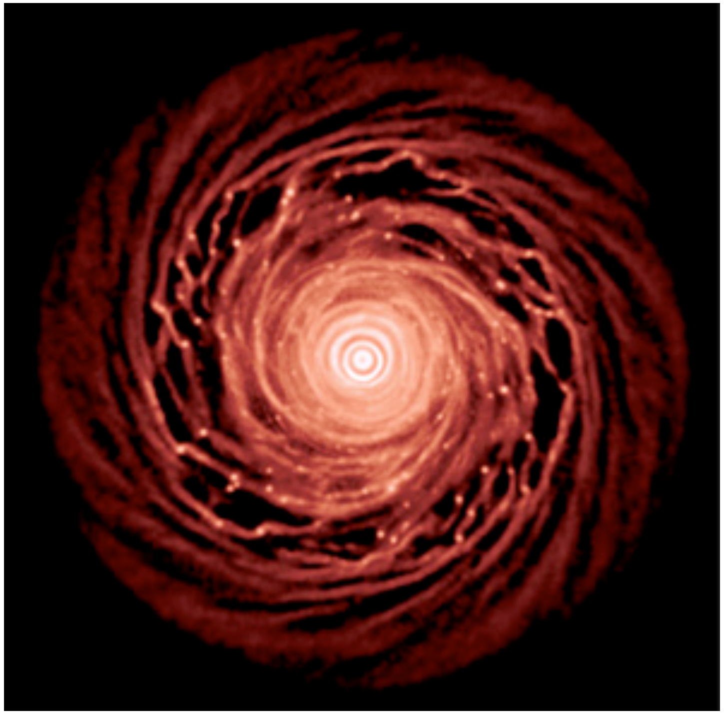
- $\tau_{\nu 0} << 1$: EW linear in N_i (all atoms absorb)
- $\tau_{\nu 0} \approx 1$: saturation; EW stalls at the Doppler width
- $\tau_{\nu 0} >> 1$: damping wings become optically thick; EW goes as $N_i^{1/2}$

Beware of saturation! If unresolved, lines look normal, but are in fact black

Rotational (Doppler) Broadening



Extending this to accretion disks in the Newtonian limit



http://jilawww.colorado.edu/research/images/accretion.jpg

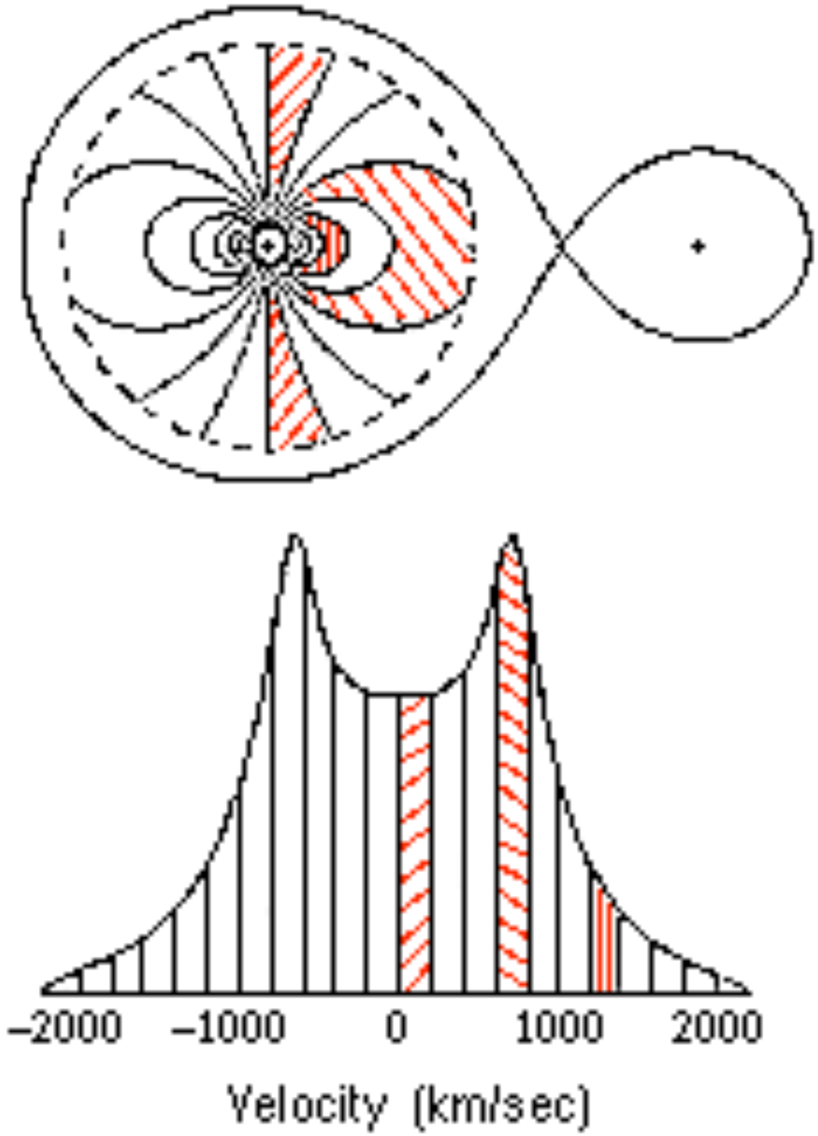
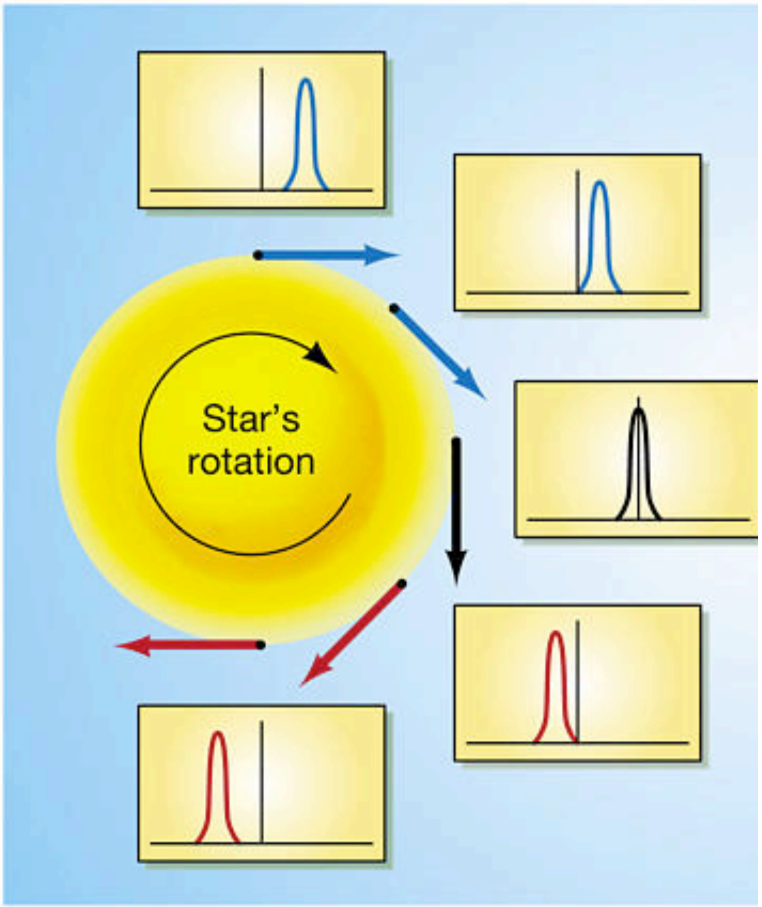
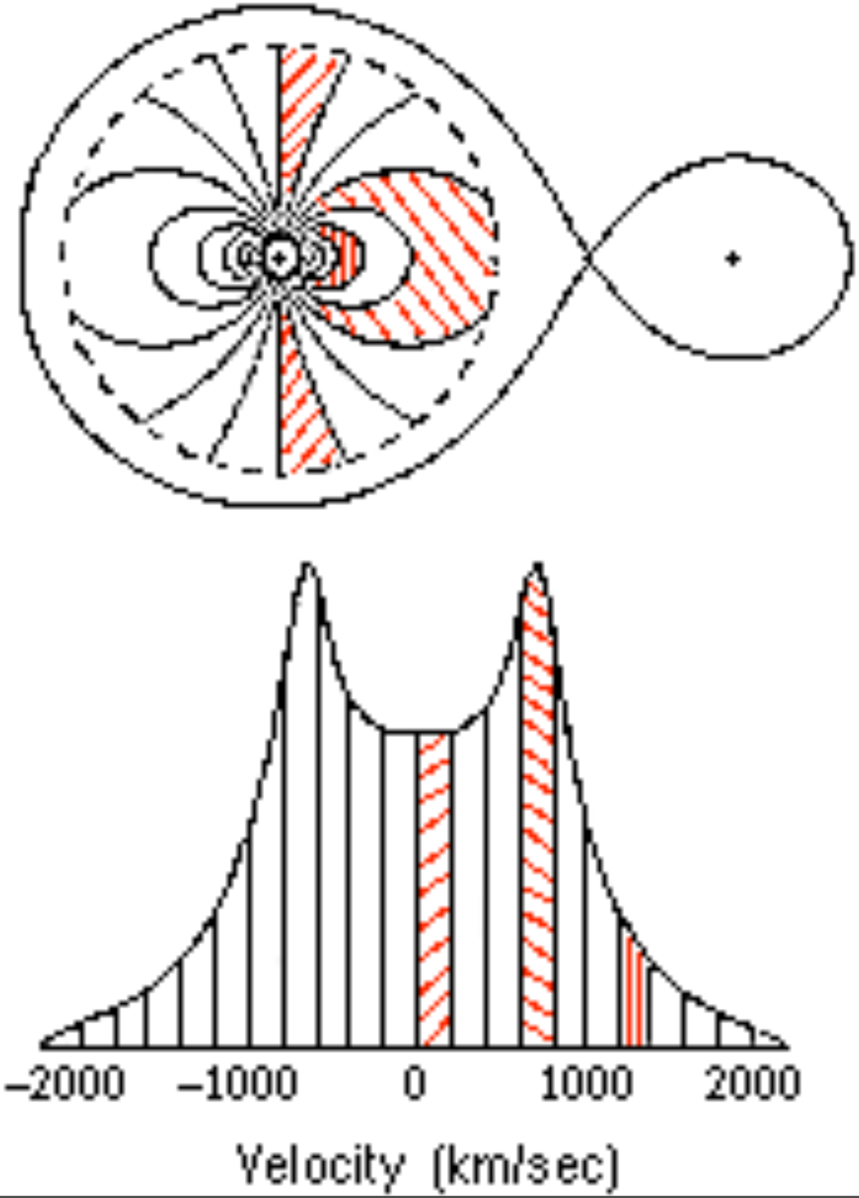


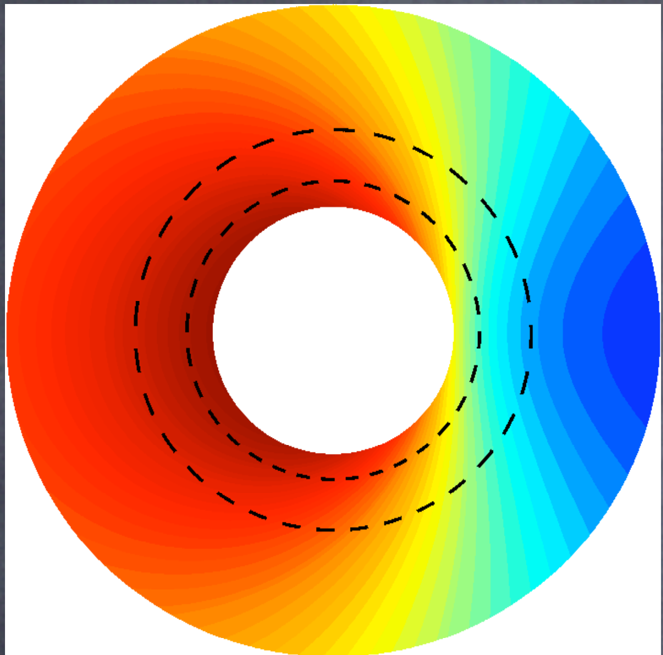
Fig. from imagine.gsfc.nasa.gov

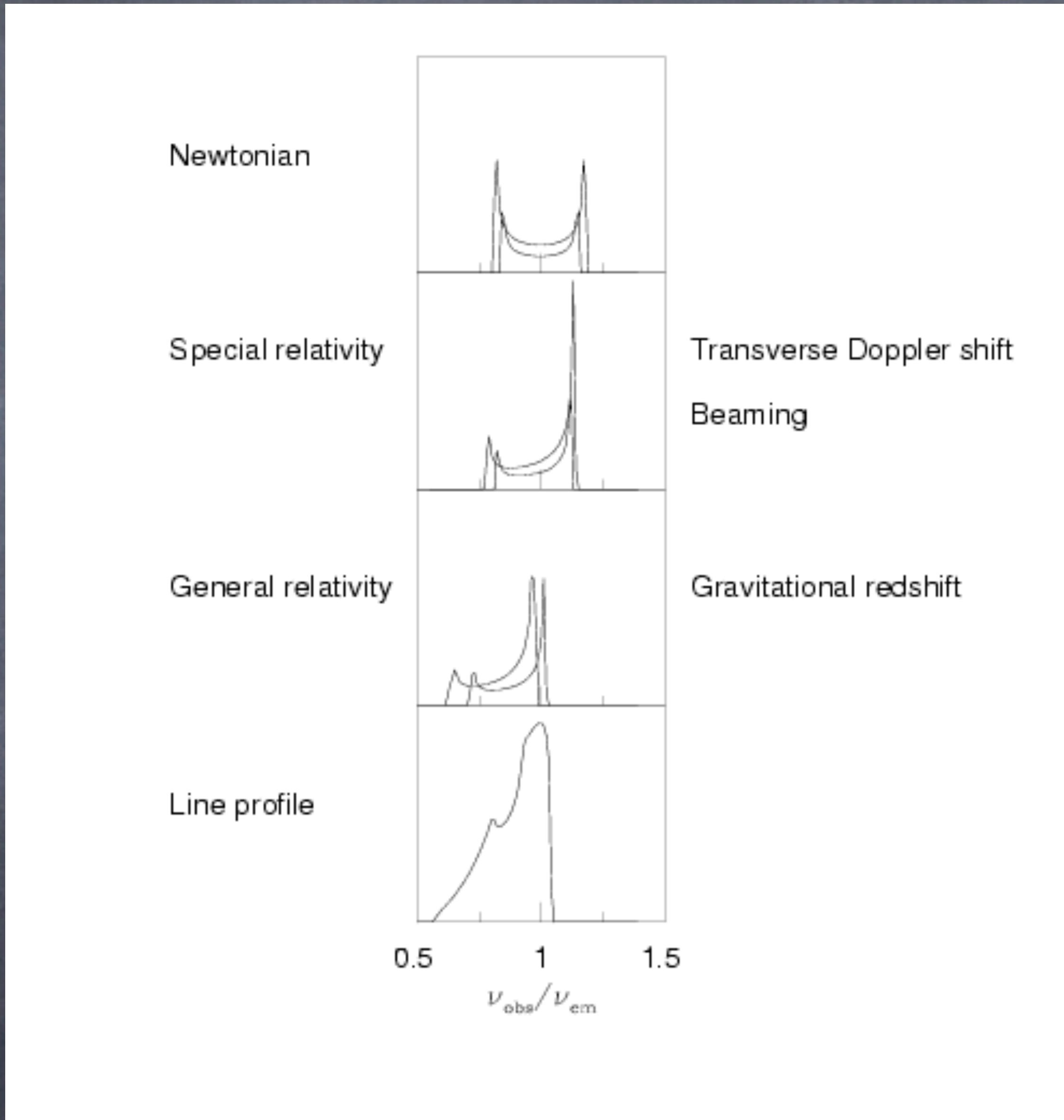
Rotational Broadening in Accretion Disks





Iron line Profiles near a Black Hole



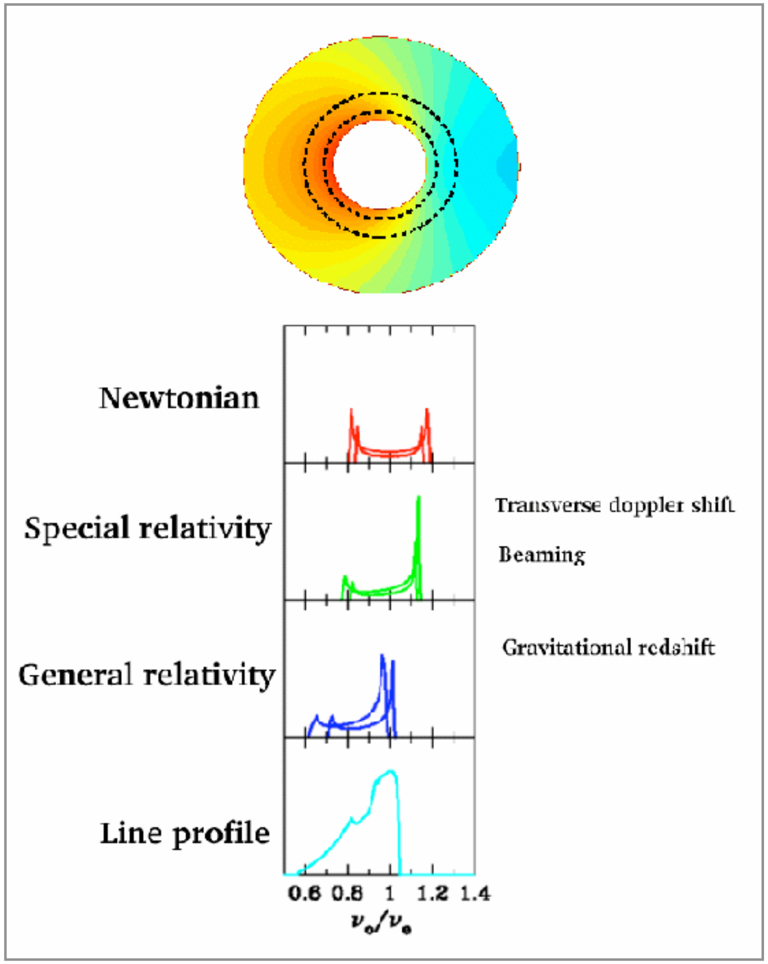


REVIEWS :

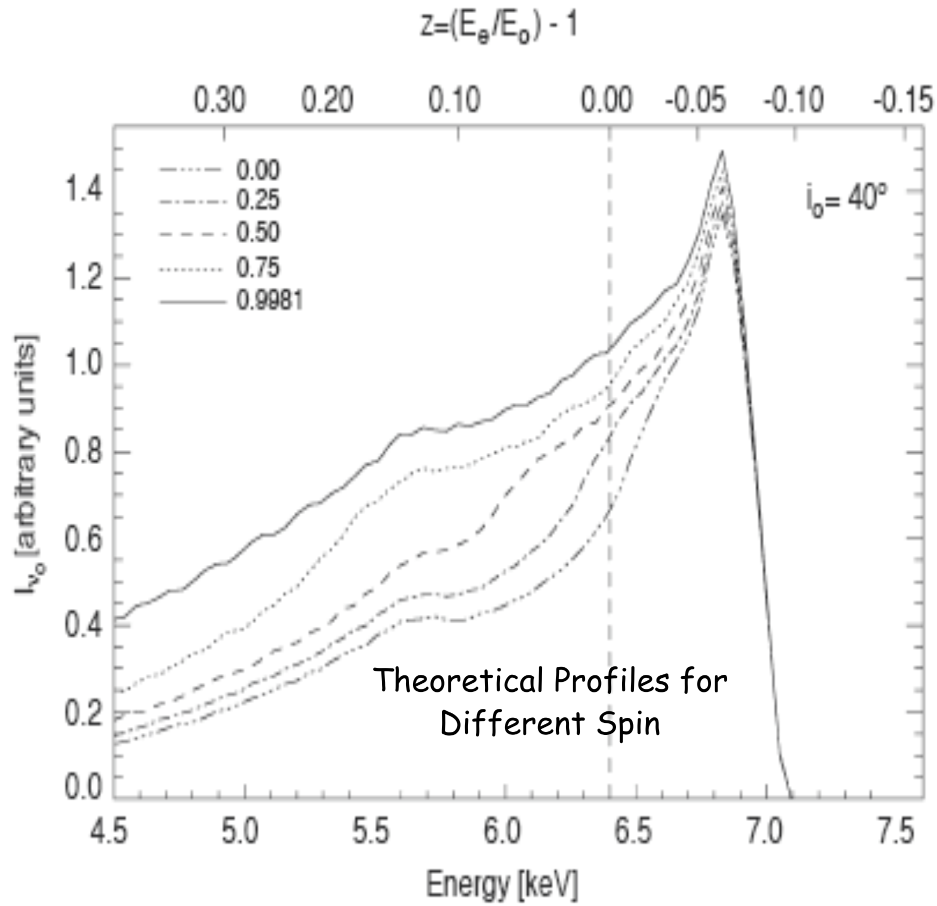
Fabian et al. 2000

Reynolds & Nowak 2003

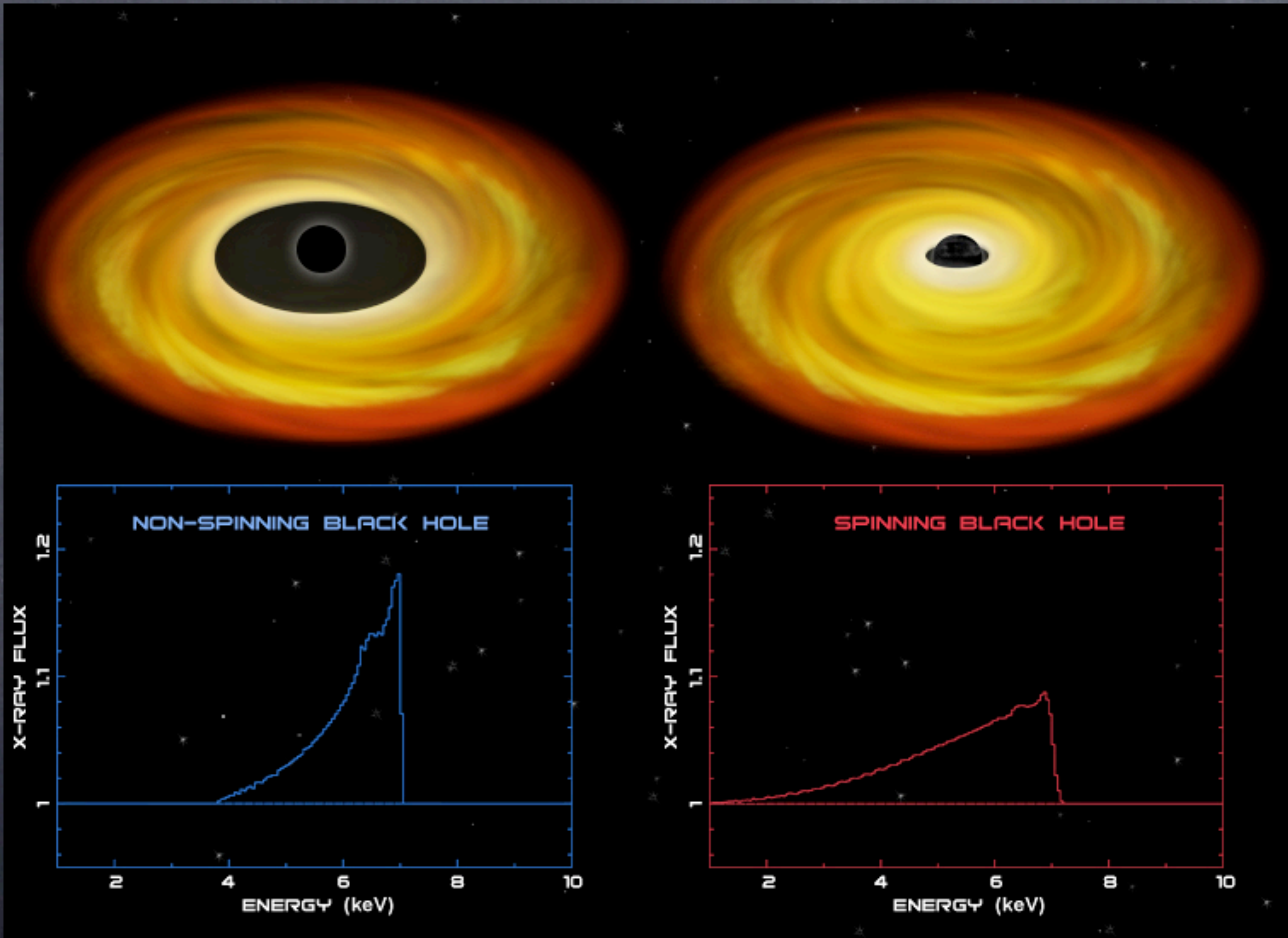
Relativistic effects imprint characteristic profile on the emission line…



Andy Young

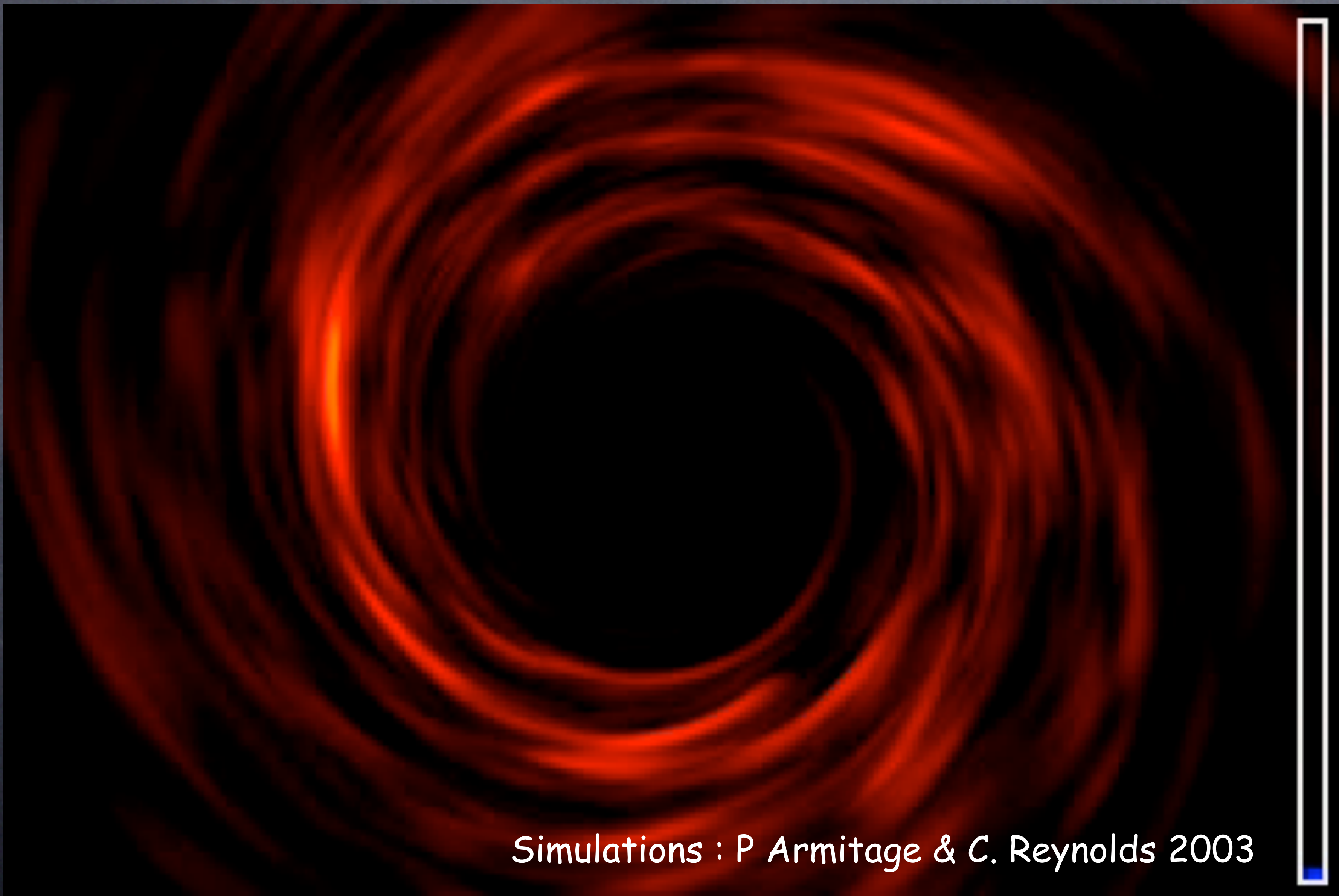


Schwarzchild vs. Kerr Black Holes

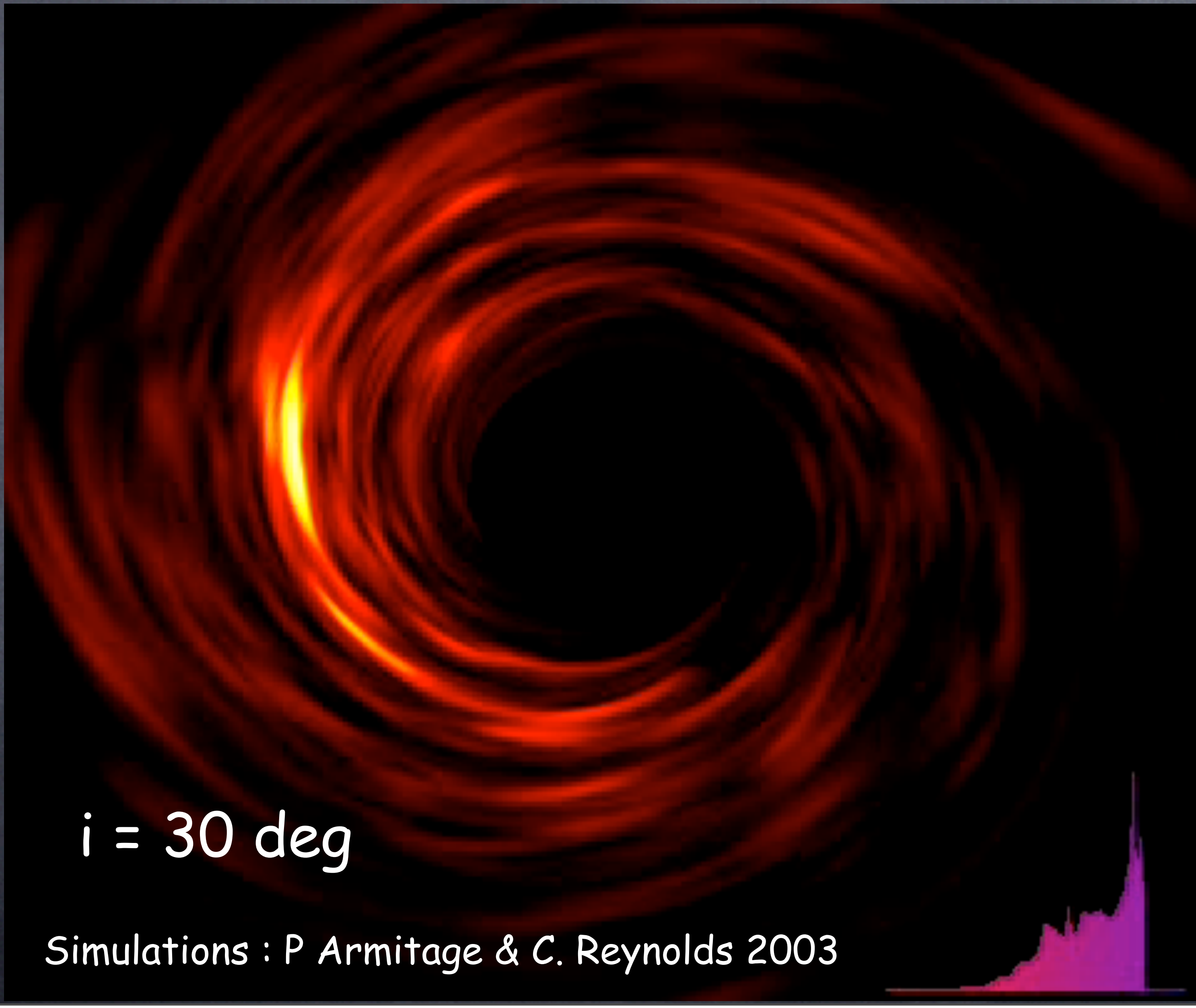


Credit : NASA/CXC/M.Weiss; Spectra: NASA/CXC/SAO/J.Miller et al.

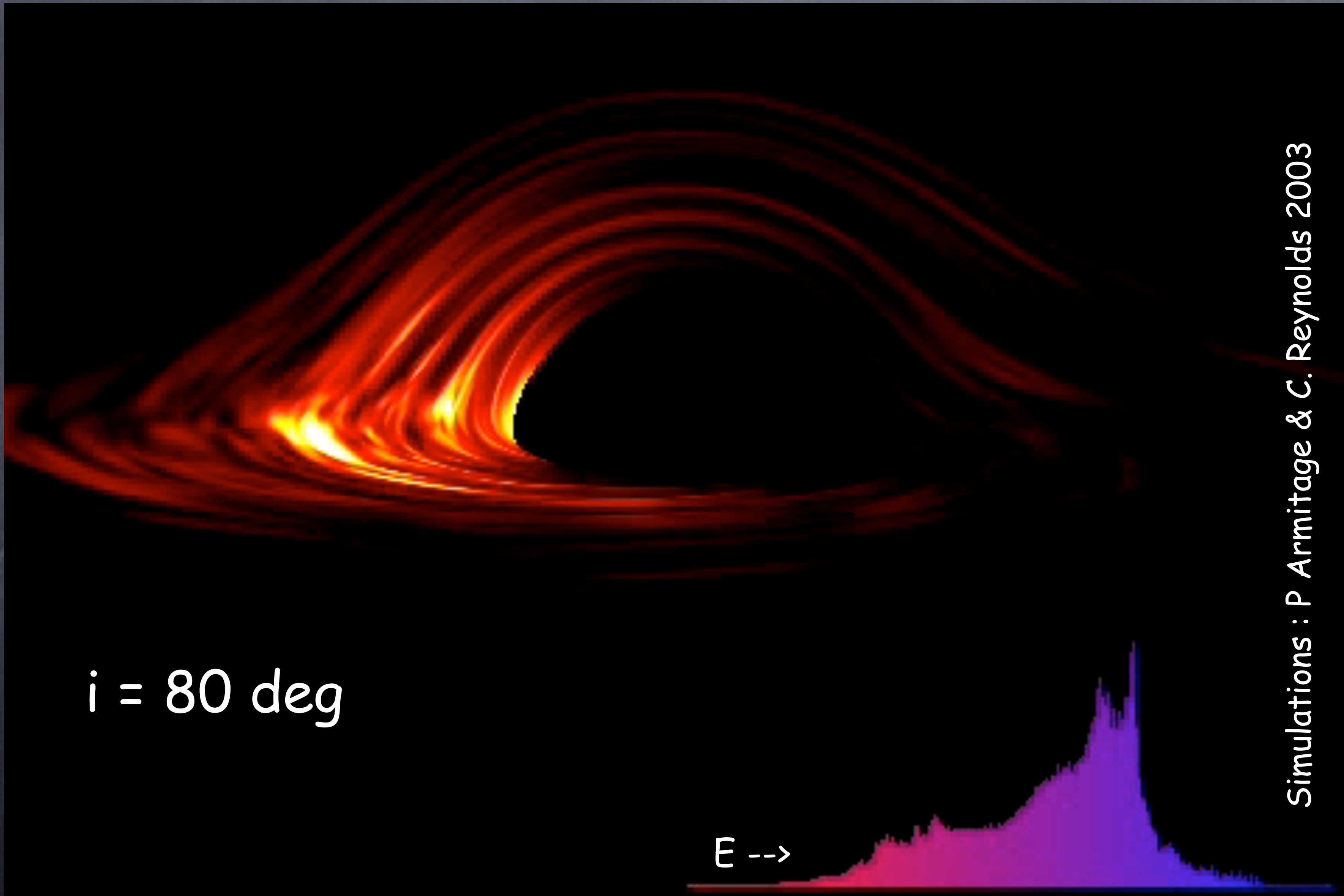
Accretion Disk Surrounding a non-rotating (Schwarzschild) black hole



Turbulent Accretion Disk Surrounding a non-rotating (Schwarzschild) black hole

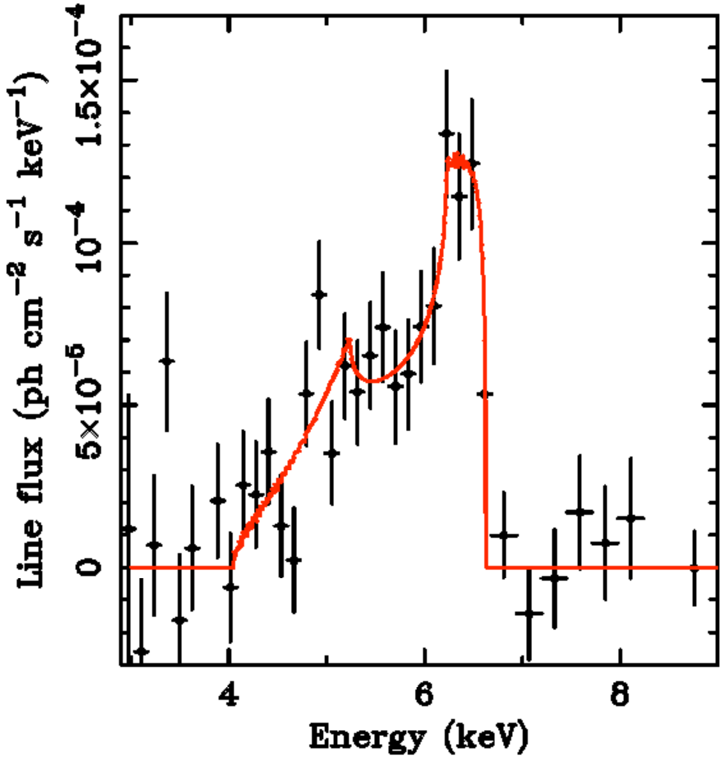


Turbulent Accretion Disk Surrounding a non-rotating (Schwarzschild) black hole



Observations of relativistic emission lines

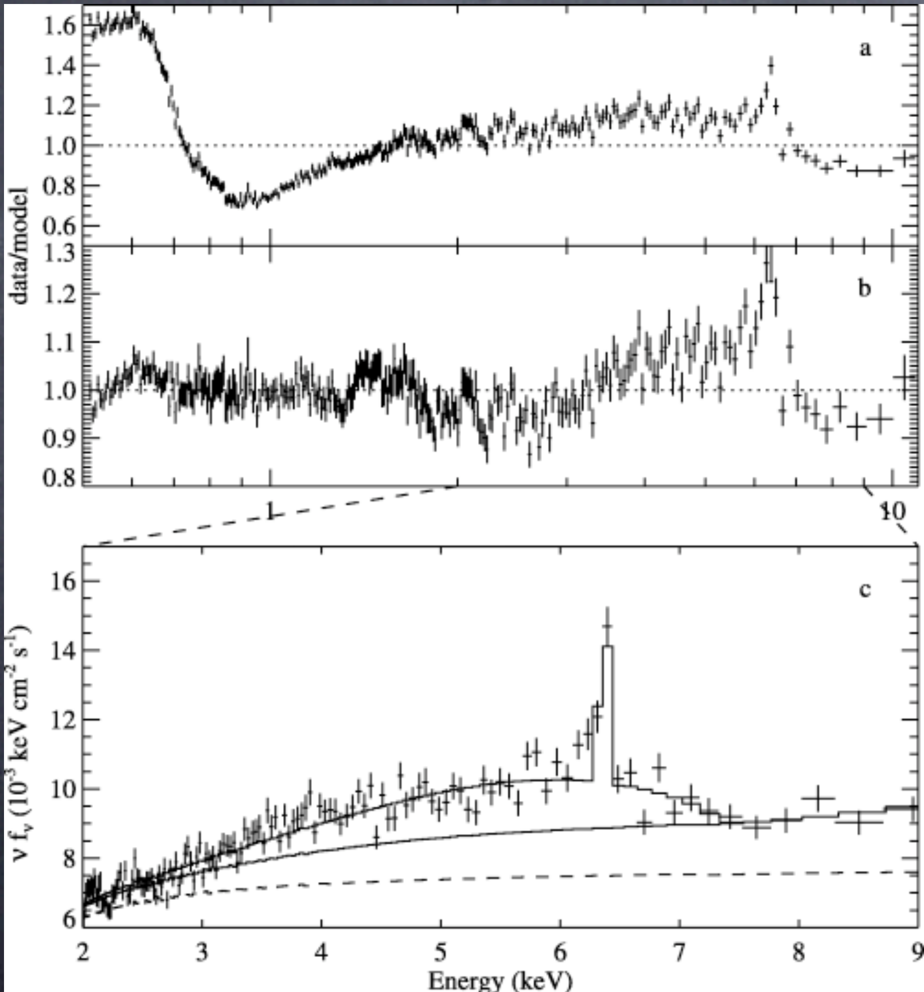
- First seen in 1994 with ASCA observatory
- 5 day observation of Seyfert-1 galaxy MCG-6-30-15
- Needed long observation to collect enough photons to form detailed spectrum



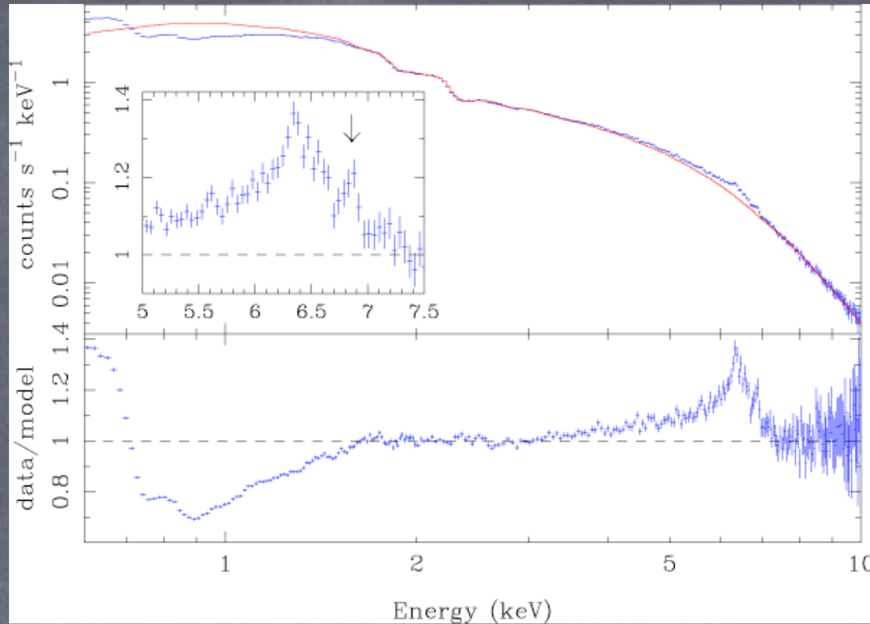
Power-law continuum subtracted
ASCA: Tanaka et al. (1995)

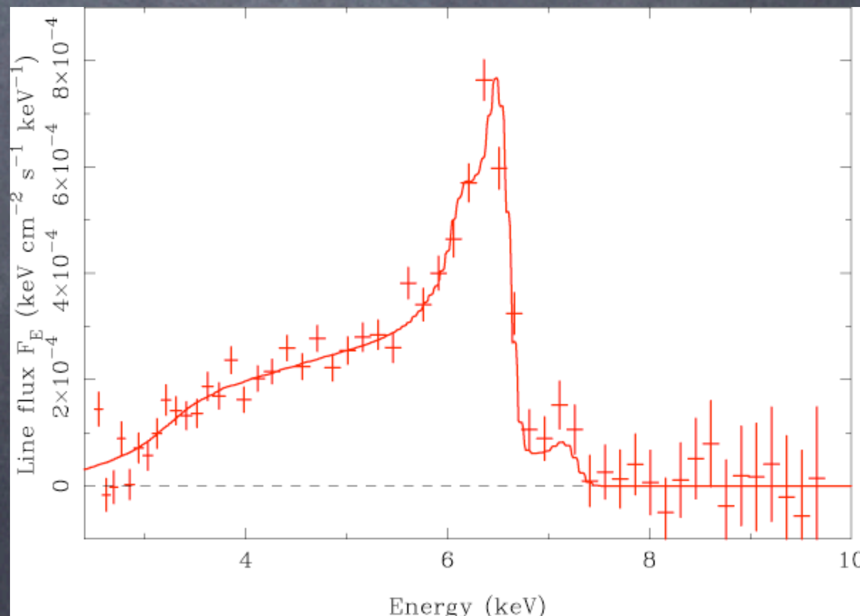
21st Century Fe line measures:

XMM-Newton View of the MCG--6-30-15 relativistic iron line



Wilms et al. 2001

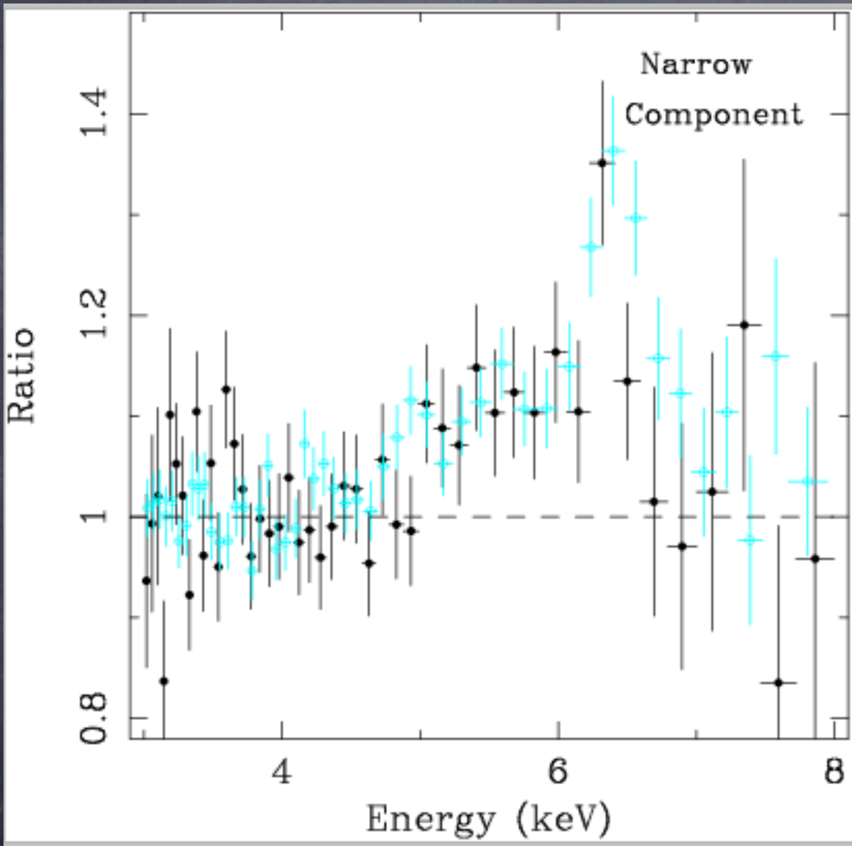




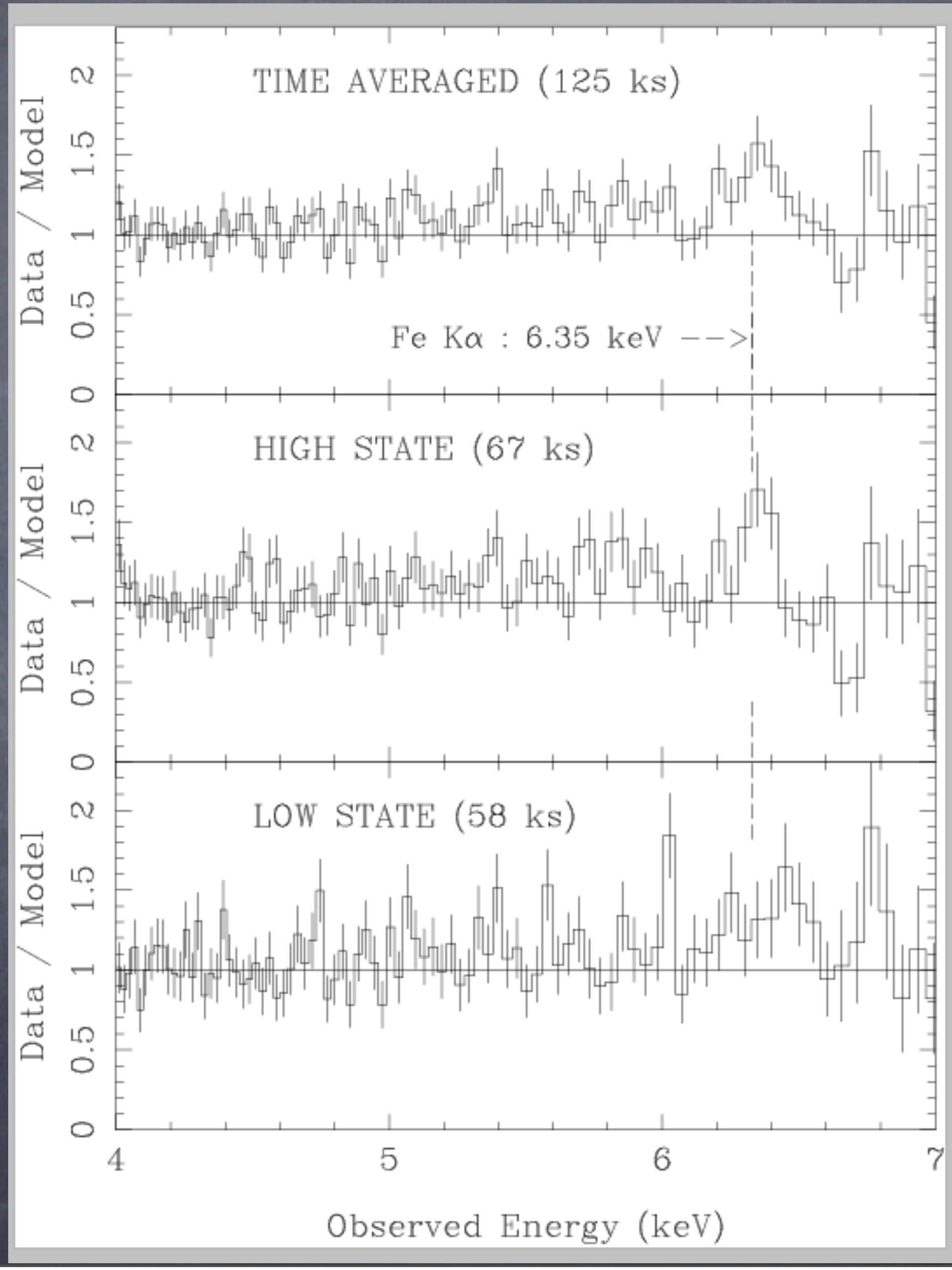
Both papers available in handout packet

Fabian et al. 2002

A high spectral resolution diagnostic of the individual narrow components of the MCG-60-3-15 Fe line

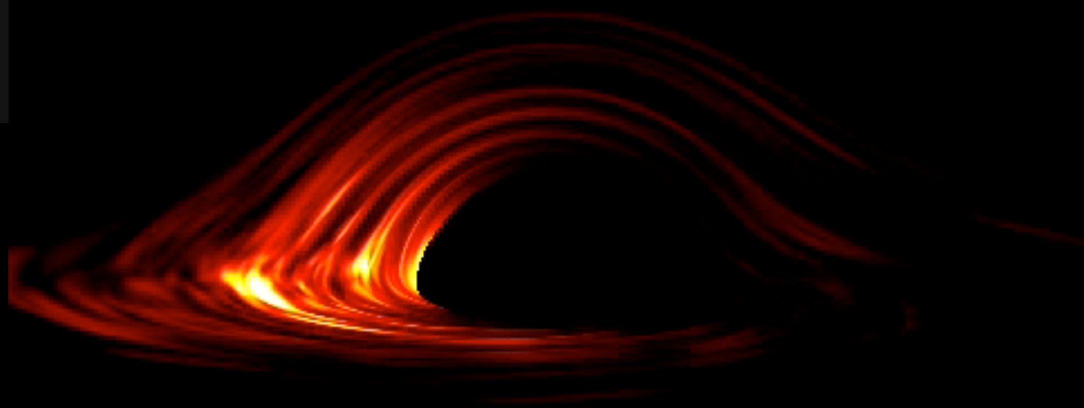


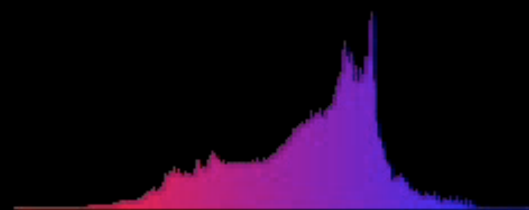
J.C Lee et al. 2002



Dynamics from line widths:
From Atomic motions to General Relativity

Motions of atoms seen in line-widths subject plasma conditions

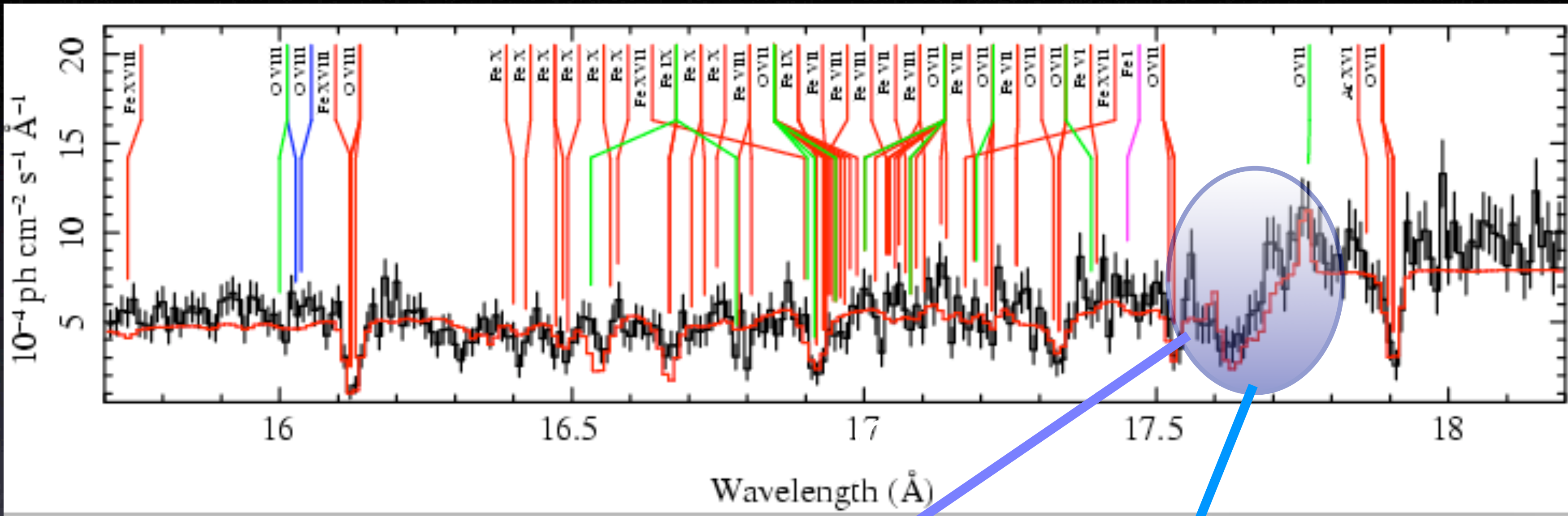




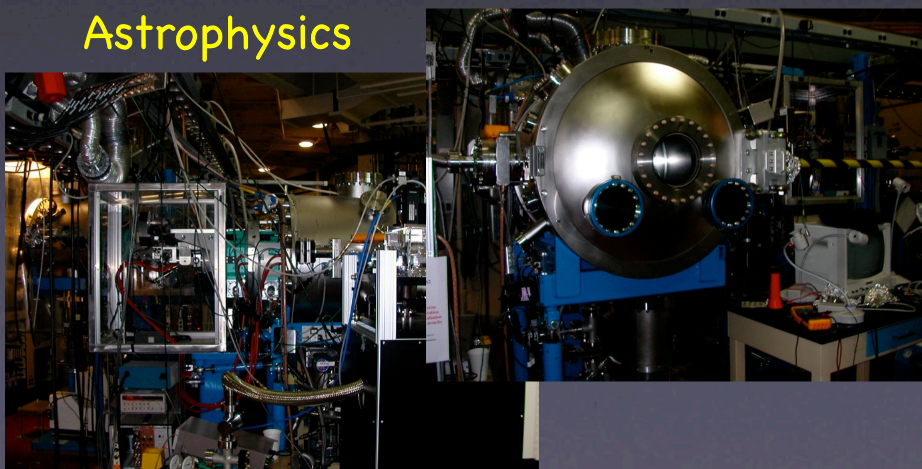
Turbulence and GR Effects

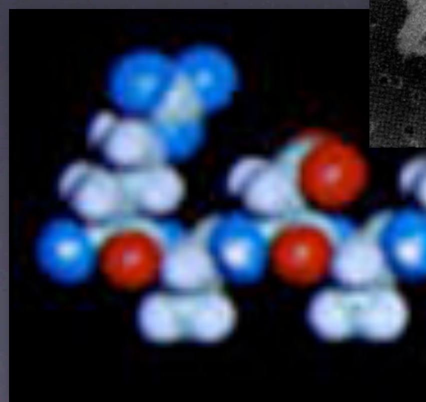
An X-ray Perspective on Determining Dust Composition

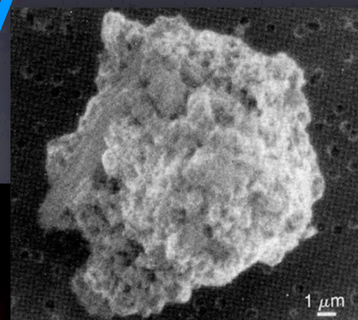
JCL with J. Xiang (Harvard), B. Ravel (NRL, ANL, NIST) , J. Kortright (LBNL)



Condensed Matter Astrophysics







Dust/Molecular Composition ?

The theory behind measuring X-ray Absorption Fine Structure (XAFS) to determine molecular/dust composition

- The photoelectric effect : X-ray photon absorbed by an electron in a tightly bound quantum core level (e.g. 1s or 2p)
  - Bound free continuum absorption → edge step
  - Isolated Atoms: Bound-bound process -> ionized lines
  - Molecule : bound-bound process → XAFS

The theory behind measuring X-ray Absorption Fine Structure (XAFS) to determine molecular composition

Fermi's Golden Rule :

initial state : an X-ray, a core electron, no photo-election

$$\mu(E) = \mu_0(E)[1+\chi(E)] \propto |< i \,|\, H \,|\, f \; >|^2$$

final state : no X-ray, a core hole, a photo-election

Fine-Structure Term :

depends ONLY on absorbing atom

change in photo-electron final state due to back-scattering from neigboring atom

$$\chi(E) = \frac{\mu(E) - \mu_0(E)}{\Delta\mu_0(E)} \propto < i \,|\, H \,|\, \Delta f \; >$$

H: interaction term - represents changing between 2 energy, momentum states

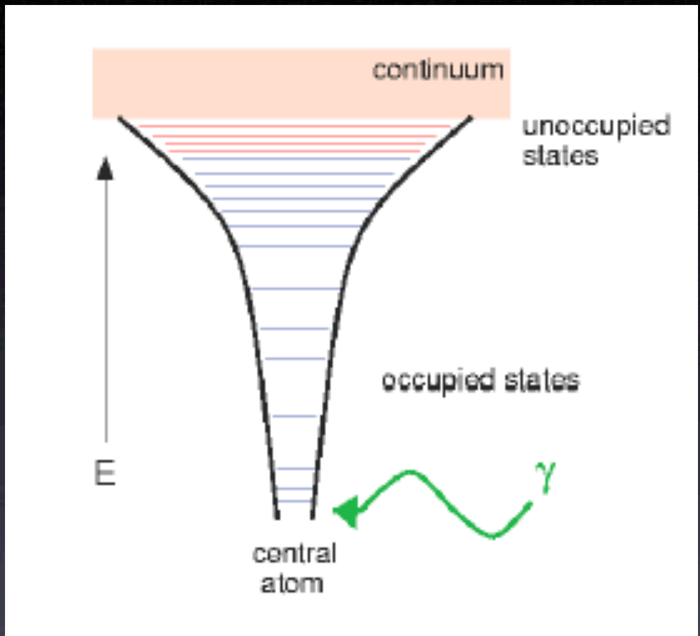
photo-electron scattering properties of neighboring atoms

The XAFS equation : represents interaction of forward scattering & backscattering photoelectron

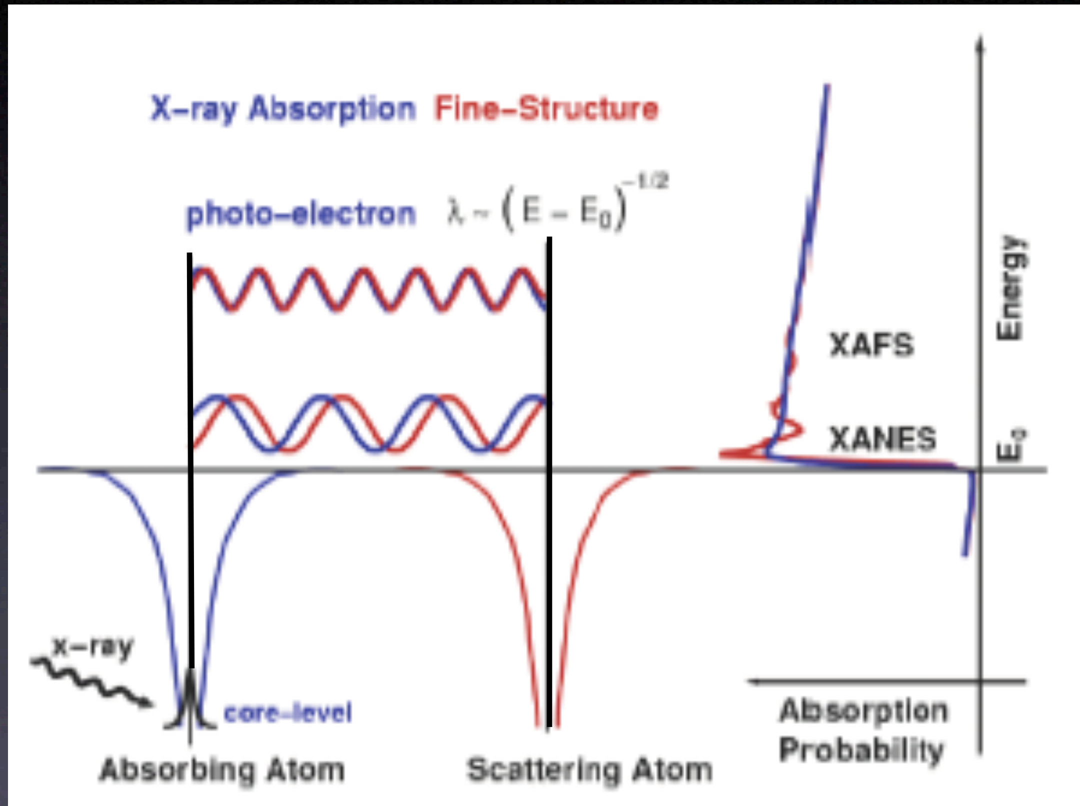
$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)}\, e^{-2k^2\sigma_j^2}}{k{R_j}^2} \sin[2kR_j + \delta_j(k)]$$

Single Scattering Approximation

XAFS Theory
Bound-bound case for CM (dust+molecules)



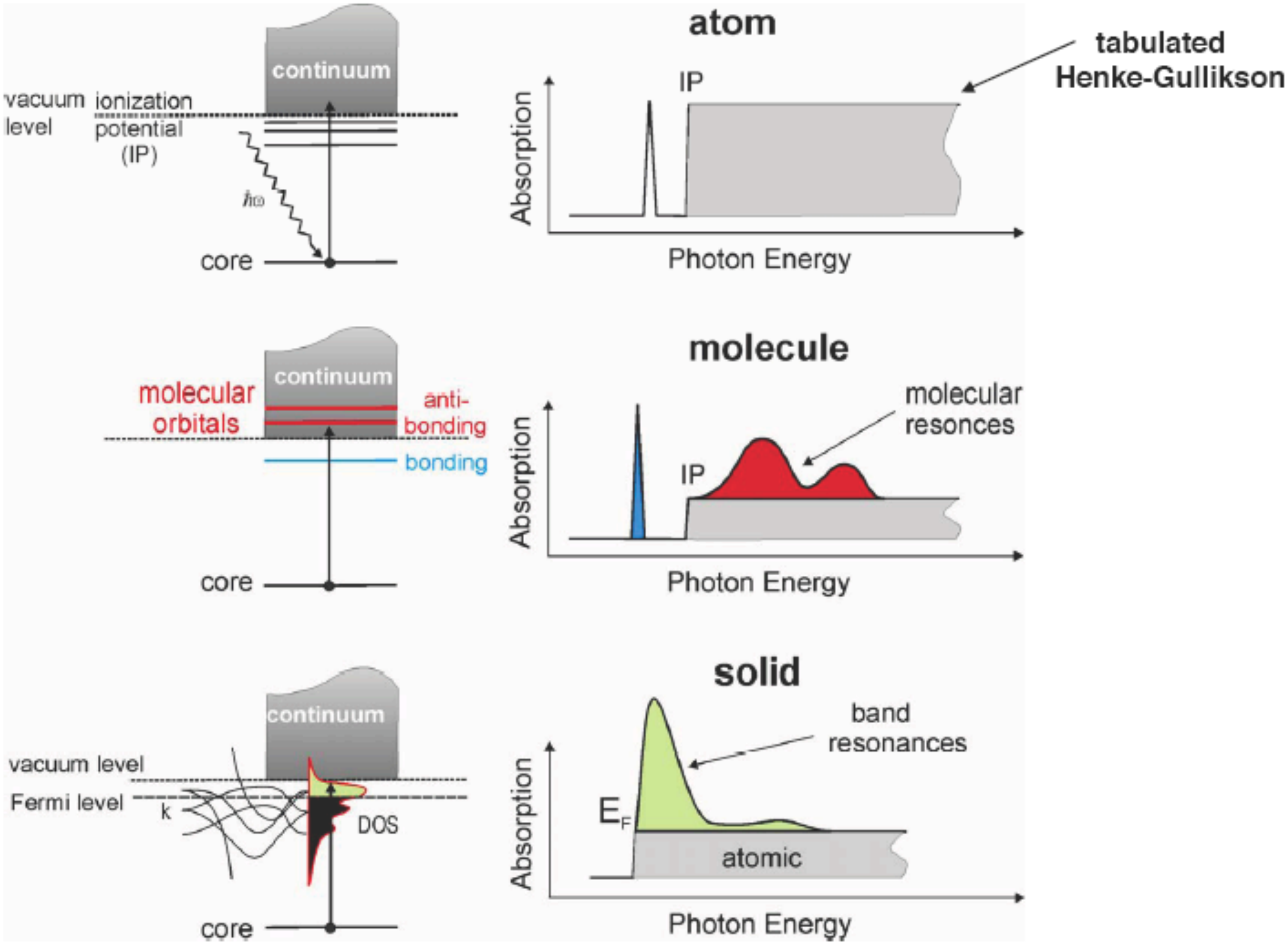
$$\mu(E) = \mu_0(E)[1 + \chi(E)]$$



Figures from "XAFS" : © 2002 Matt Newville

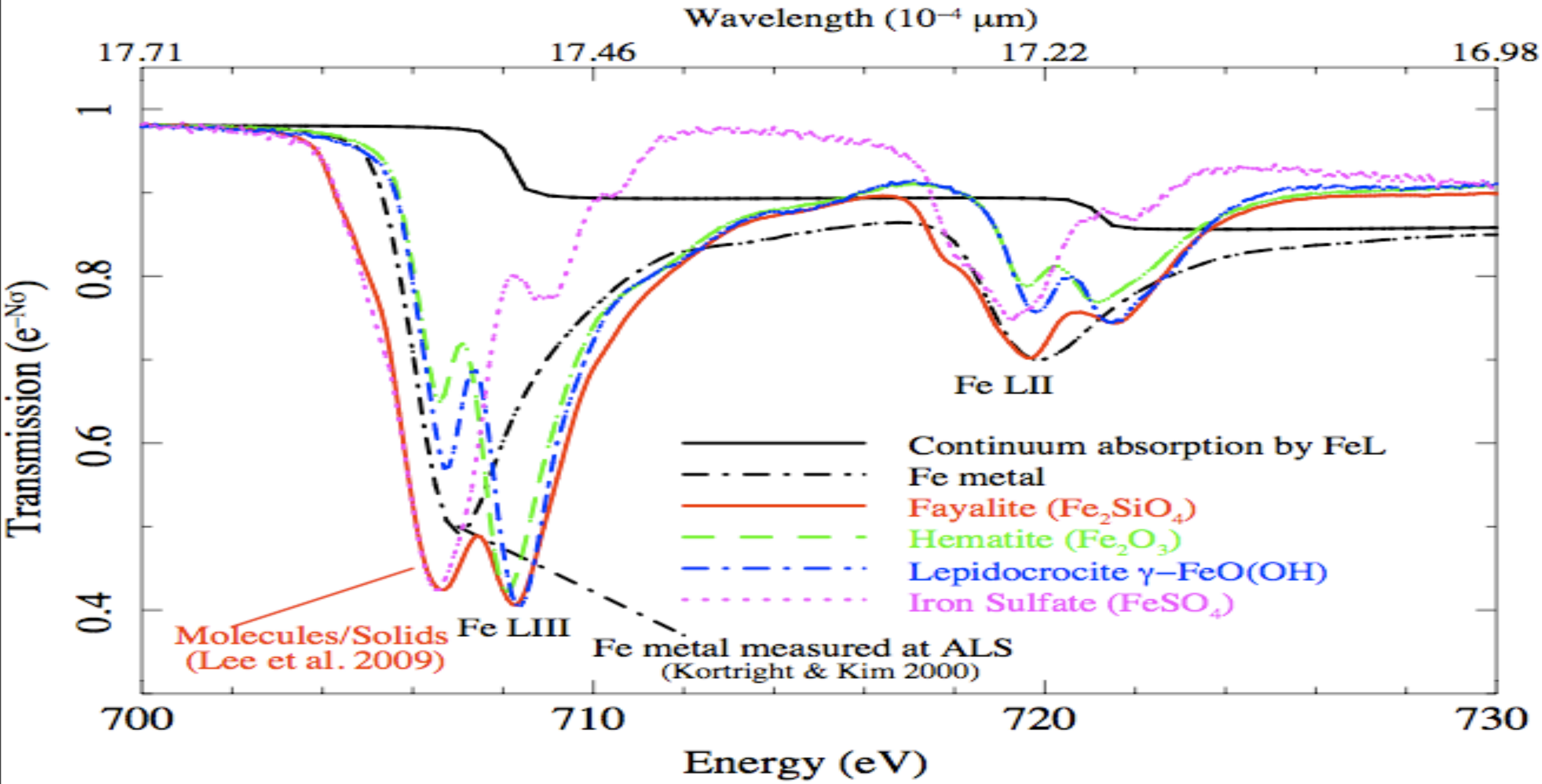
The amplitude of the back-scattered photo-electron at the absorbing atom will vary with energy --> oscillations in μ(E) --> XAFS

X-ray Absorption Spectra in a Nutshell



From Stohr lecture: www-ssrl.slac.stanford.edu/stohrgroup

Dust will imprint structure near photoelectric edges

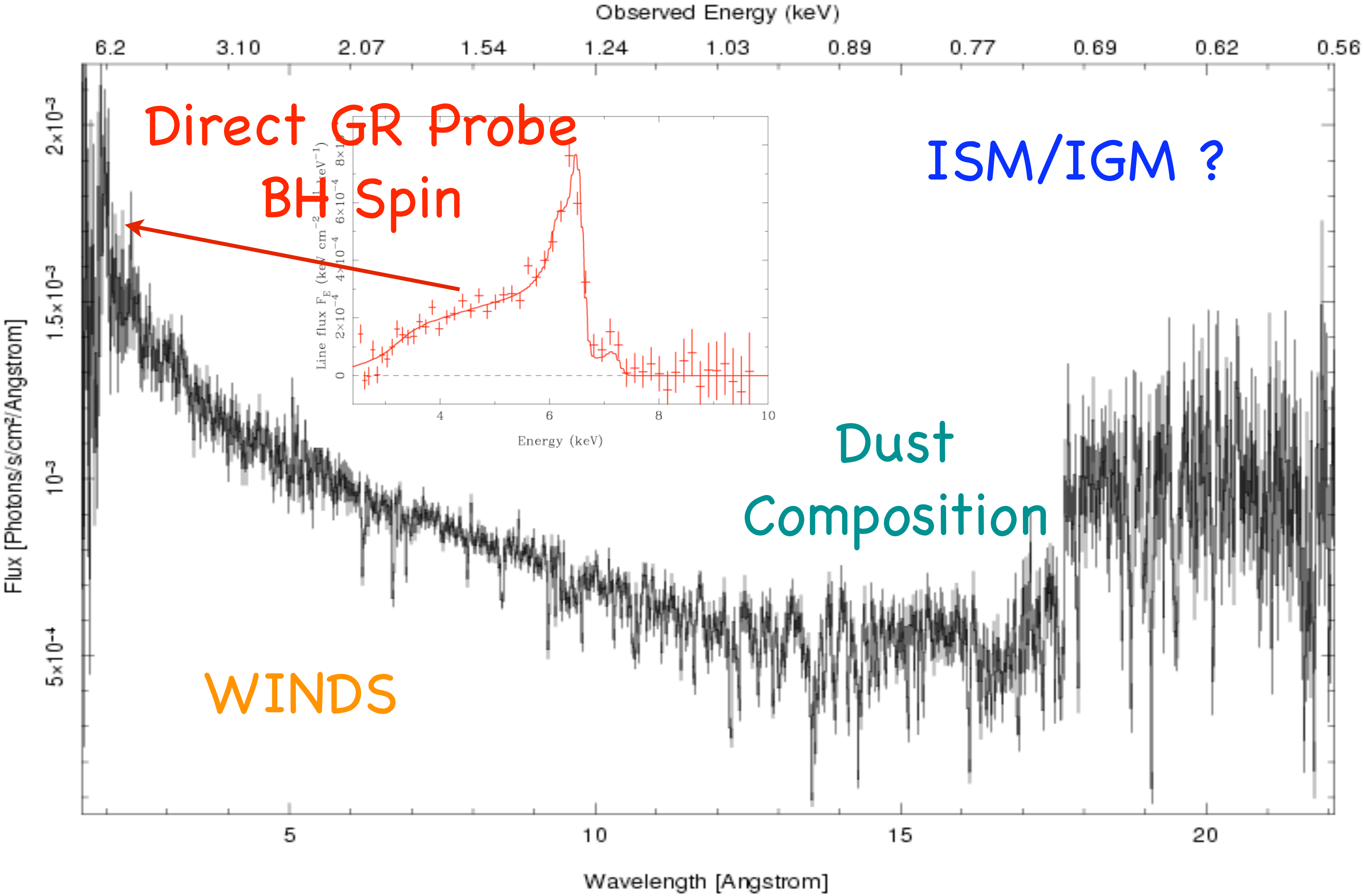


For details on theory & astrophysics applications:

Lee & Ravel 2005

Lee et al. 2009, in press

The Rich Information Content in an X-ray Spectrum

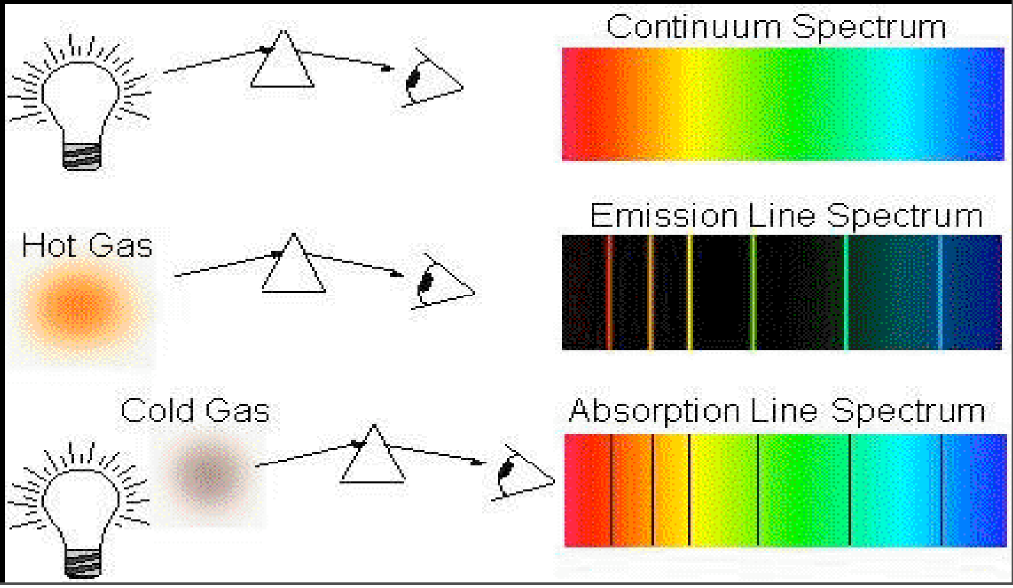


Using Quantum Mechanics to do Astrophysics

- Atoms can be identified by their unique set of spectral lines
- Relative line strengths dependent on temperature, density
- Emission/Absorption: dependent on viewing geometry
- Use these properties to figure out dynamics

Gas temperature and viewing angle dictates what we see:

- continuum radiation,
- emission lines, or
- absorption lines



Conclusions

Although moderately complex, there are relatively few processes that dominate X-ray emission; analyzing the observed spectrum from each can reveal the underlying parameters. These processes are:

- Line emission
    - Collisional ⇒ temperature, abundance, density
    - Photoionized ⇒ photoionization parameter, abundance, density
- Absorption ⇒ abundance, density, velocity
- Continuous Spectrum

  Synchrotron emission ⇒ relativistic electrons, magnetic field

  Inverse Compton scattering ⇒ relativistic electrons

  Blackbody ⇒ temperature, size of emitting region / distance^2

Plasma Codes

Understanding a collisional plasma requires a collisional plasma model. Since even a simple model requires considering hundreds of lines, and modern codes track millions, most people select one of the precalculated codes:

Code	Source
Raymond-Smith	ftp://legacy.gsfc.nasa.gov/software/plasma_codes/raymond
SPEX	http://saturn.sron.nłgenerałprojects/spex
Chianti	http://wwwsolar.nrl.navy.miłchianti.html
ATOMDB	http://cxc.harvard.edu/ATOMDB

The calculated spectrum is also known as APEC, and the atomic database is called APED.

From Randall Smith Lecture @ xrayschool.gsfc.nasa.gov

Plasma Codes

The collisional plasma models available in XSPEC or Sherpa are:

apec	ATOMDB code; good for high-resolution data
raymond	Updated (1993) Raymond-Smith (1977) code
meka	Original Mewe-Kaastra (Mewe *et al*. 1985) code; outdated
mekal	Mewe-Kaastra-Liedahl code (Kaastra 1992); new Fe L lines
c6mekal	mekal with an polynomial EM distribution
equil	Borkowski update of Hamilton, Sarazin & Chevalier (1983)
nei	Ionizing plasma version of equil
sedov	Sedov (SNR) version of equil
pshock	Plane parallel shock version of equil

Variable abundance versions of all these are available.

Individual line intensities as functions of T, n, etc. are not easily available (yet) in either XSPEC or Sherpa.

From Randall Smith Lecture @ xrayschool.gsfc.nasa.gov

Photoionized Plasma Codes

Understanding a photoionized plasma requires a plasma model plus a physical model of the system:

- Illuminated slab of gas
- Torus with central source
- Disk with 'light bulb' above it
- Central source surrounded by small absorbers
- etc...

Code	Website
XSTAR	http://heasarc.nasa.gov/lheasoft/xstar/xstar.html
CLOUDY	http://www.nublado.org/
Titan	http://Vo.obspm.fr:8888/simulation/ (in progress?)
Mocassin	http://hea-www.harvard.edu/~bercolano/

From Randall Smith Lecture @ xrayschool.gsfc.nasa.gov

Atomic Codes

HULLAC (Hebrew University / Lawrence Livermore Atomic Code) : Fast, used for many APED calculations, not generally available.

R-Matrix : Slow, used for detailed calculations of smaller systems of lines, available on request but requires months to learn.

FAC (Flexible Atomic Code) : Fast, based on HULLAC and written by Ming Feng Gu

From Randall Smith Lecture @ xrayschool.gsfc.nasa.gov

A few parting words

- There is a lot of Physics in the Lines
  - most probable transitions strongest
  - line blends common
- Think critically about model fits
  - Plasma codes have ~10% error on line strengths
  - Line energies differ depending on databases, especially more difficult transitions
- $\chi^2_n \sim 1$ **not** a useful gauge for a high resolution spectrum -- understand the physics