# Emission I:
# Atomic Physics for X-ray Astronomy

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# Introduction

## Some Simplifications:

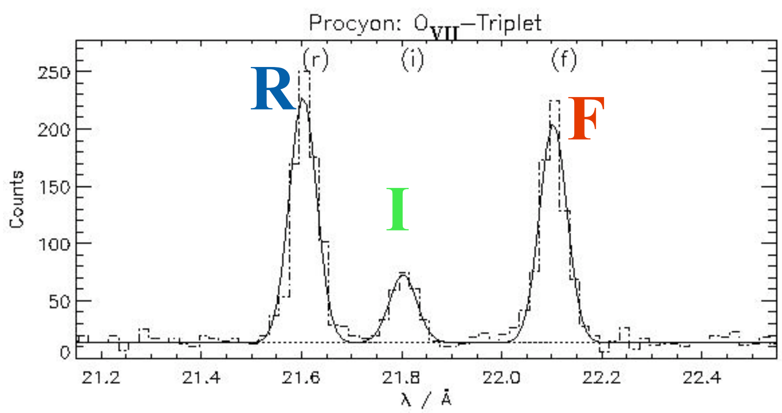
- **Atoms only**: Molecules (and dust grains) are only observable in absorption X-ray spectra with difficulty.
- **No nuclear transitions**: By definition these are $\gamma$-rays.
- **No three-body transitions**: Except in the densest regions, these are astrophysically unimportant.
- **No metal-metal collisions**: X-ray emitting plasmas have densities so low that even He-atom collisions are unimportant.
- **No neutral plasmas**: Most X-ray emitting plasmas are at least partially ionized, so $n_e \approx n_H$

# Important Processes In X-ray Plasmas

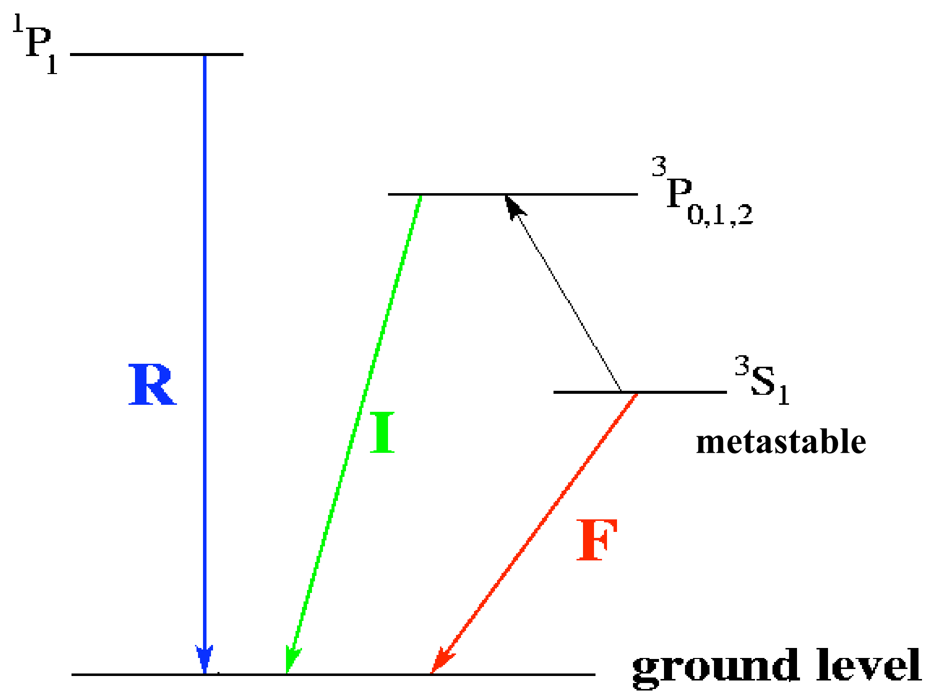
- Ionization
  - Electron/Proton Collisions
  - Electron/Photon (Photoionization)
  - Innershell ionization
- Recombination
  - Radiative
  - Dielectronic
  - Charge Exchange
- Excitation/Decay
  - Electron/Proton Collisions
  - Photoexcitation
  - Radiative Decay

# Energy Levels

**R: resonance line (permitted, w)**
**I: Intercombination line (x+y)**
**F: Forbidden line (z)**




Ness et al. (2001)




**Gabriel & Jordan (1969):**

¬ **Density:** $R(n_e)$ = **Forbidden** / **Intercombination**

¬ **Temperature:** $G(T_e)$ = **(F + I)** / **Resonance**

**First widely used for solar plasma diagnostics.**

**Now: extra-solar objects: collisional (e.g., stellar coronae), photo-ionization (e.g., AGN, X-ray binaries), out-of-equilibrium (e.g., SNR)**

# Energy Level Descriptions

Energy levels are most frequently given in LS-coupling :

$$n_1 l_1\ n_2 l_2\ \ldots\ {}^{2S+1}L_J$$

H-like: 1s $^2S_{1/2}$, 2p $^2P_{1/2}$, 2p $^2P_{3/2}$, 4d $^2D_{5/2}$

He-like: $1s^2$ $^1S_0$, 1s2p $^1P_1$, 1s2p $^3P_2$, 1s4d $^3D_3$

However, when atoms become more complex, this simple system breaks down. Sometimes both the core structure and the outer electron structure is given, as in :

O-like: $1s^2\ 2s^2\ 2p^4\ {}^3P_2$, $2s^2 2p^3(^4S)$ 3s $^5S_2$, $2s^2 2p^3(^2D)$ 3d $^1F_3$

More commonly, strong transitions pick up "shorthand" names. Some of the strongest Fe XVII (Ne-like) lines are known simply as the 3C (15.01Å), 3D (15.26Å), 3F (16.78Å), 3G (17.05Å) and M2 (17.10Å) lines.

# How do we identify emission lines?

**By matching the observed line to the expected line**
(based on theoretical or laboratory measurements)

Problems:

- Unless the analysis is done line-by-line (ie, not in XSPEC or *Sherpa*), taking wavelength errors (if available) into account is nigh unto impossible.
- Not all wavelengths are known from lab measurements.
- How good are purely theoretical wavelengths? It depends on the ion involved, but in general a good calculation is accurate to 1%

# Is 1% Accuracy Adequate?

Only if you don't care about Doppler shifts:

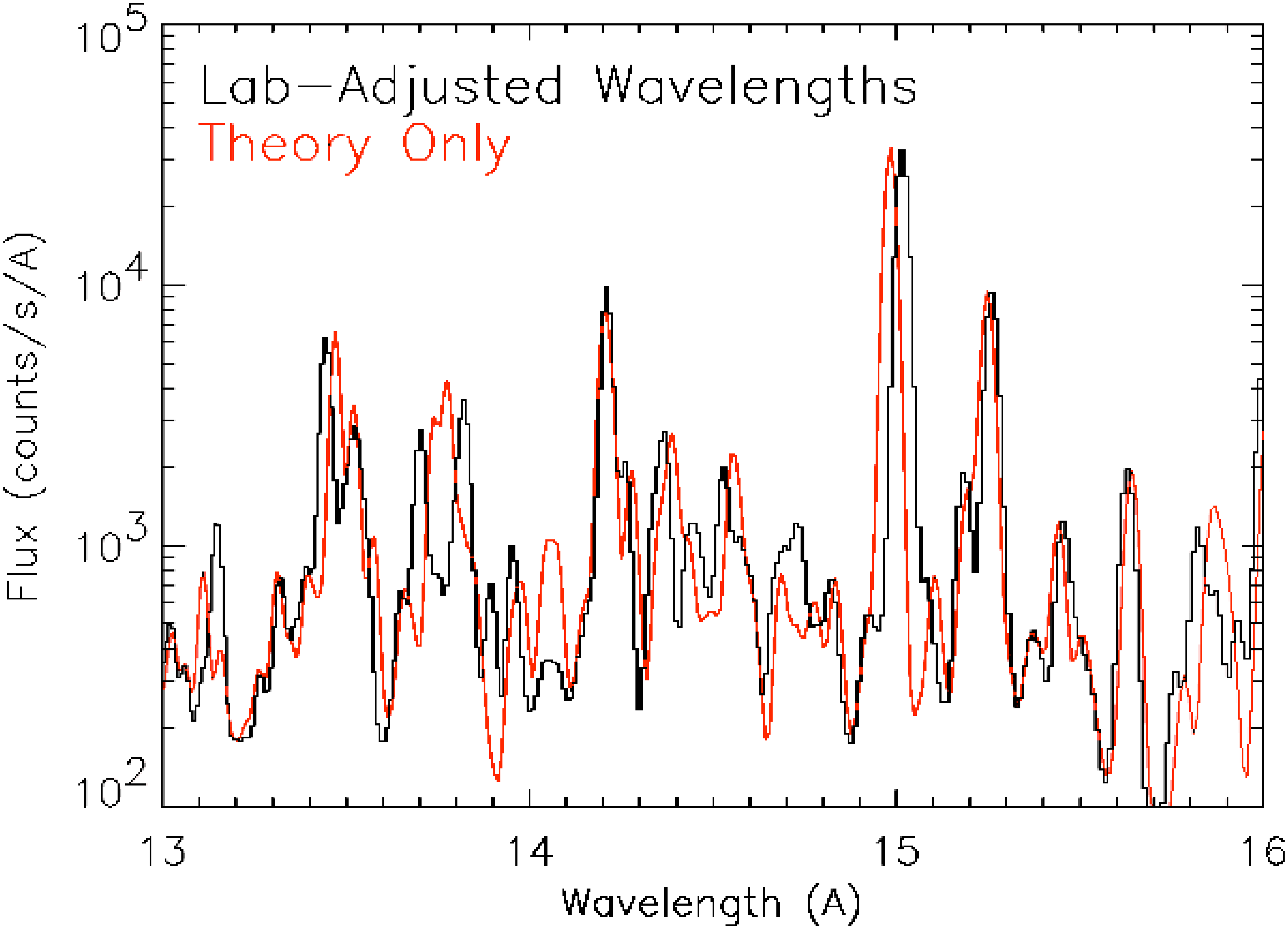
$$\frac{v}{c} = \frac{\Delta\lambda}{\lambda} \rightarrow v = 0.01c = 1000\,\mathrm{km/s}$$

Lesson:

**If it matters to your analysis, know what's in your model!**

The biggest difference between the Mekal and APEC collisional plasma models is that APEC has more accurate wavelengths, since it was designed with high-resolution detectors in mind.

# Laboratory measurements are necessary!



# Radiative Transitions

A "radiative transition rate" (or "Einstein A value") is the rate (in $s^{-1}$) at which an excited ion (state j) will transition to a lower energy state (k). This is related to the oscillator strength $f_{kj}$ by:

$$A_{jk} = 8\pi^2 \left(\frac{g_k}{g_j}\right) f_{kj} \left(\frac{r_e}{c}\right) \nu_{jk}^2$$

where $g_k$ is the statistical weight of the k'th level. We can plug in some numbers here to get:

$$A_{jk} = 1.7 \times 10^{15} \mathrm{s}^{-1} \left(\frac{g_k}{g_j}\right) f_{kj} \Delta E_{keV}^2$$

So transition rates for allowed (f ~ 1) X-ray transitions are rapid. Forbidden transitions can have ***much*** smaller values; the O VII 1s2s $^3S_1 \rightarrow 1s^2\ ^1S_0$ transition is only ~ 1000 $s^{-1}$.

## Radiative Transitions

These rates are crucial to photoionized plasmas, or when calculating if a line is optically thick.

It is less important when working with collisional plasmas, although **density diagnostics** result from the relative rates of collisional (de)excitation and radiative decay.

Transition rate data are available on WebGUIDE:

http://asc.harvard.edu/atomdb/WebGUIDE/index.html

# Two Photon Transitions

Some transitions are absolutely forbidden, and as a result transition via the so-called "two-photon" transition. The only two of importance for X-ray astronomy are:

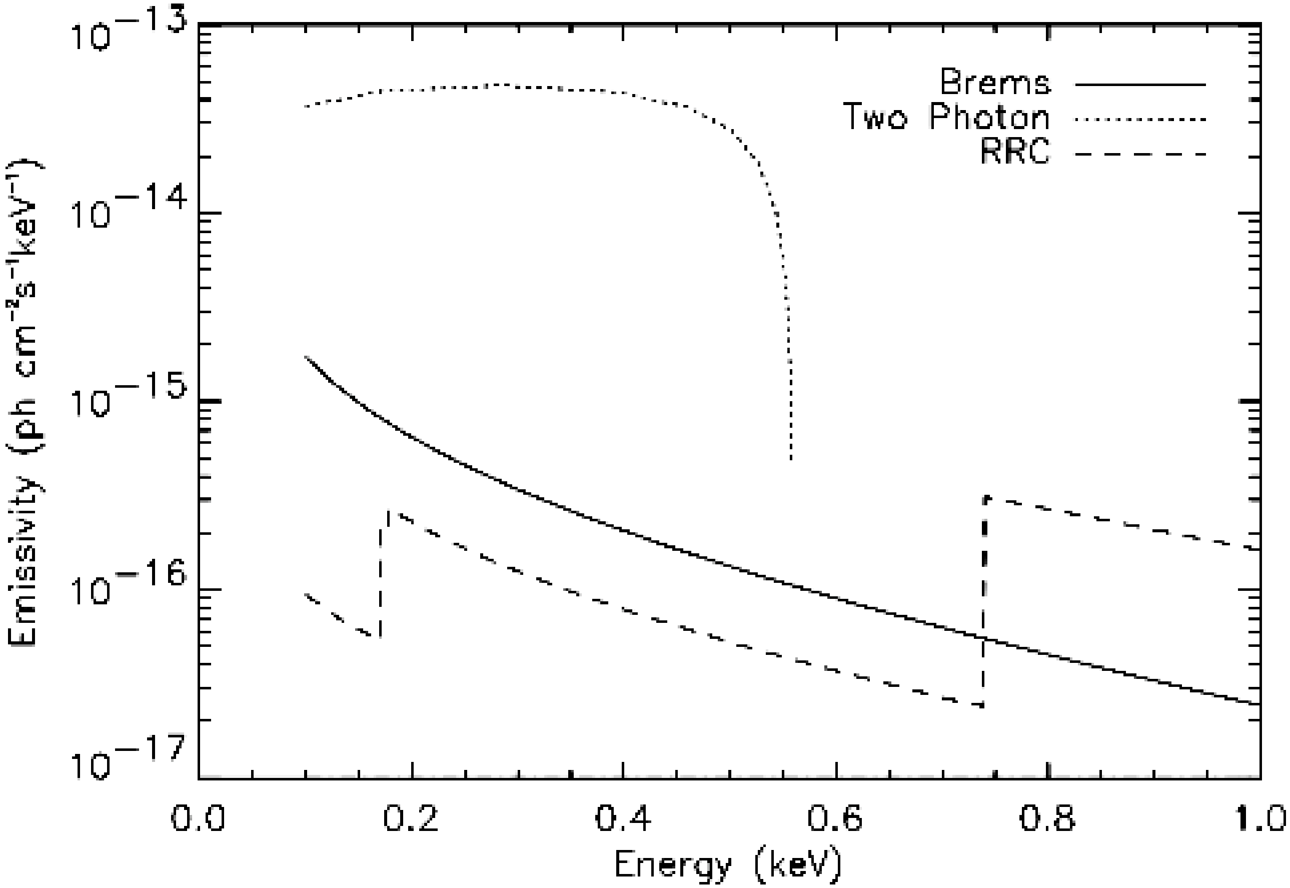
$$\text{H-like} \quad : 2s\ ^2S_{1/2} \rightarrow 1s\ ^2S_{1/2}$$

$$\text{He-like} : 1s2s\ ^1S_0 \rightarrow 1s^2\ ^1S_0$$

Curious fact: The A values for these transition in Oxygen are 8425 and $2.31\text{x}10^6$/s. The A value for the O VII "forbidden" transition is 1044/s! There is a two-photon transition from the forbidden level, but its A value is << 1/s.

# Two Photon Transitions

The O VII two-photon transition : 1s2s $^1S_0 \rightarrow 1s^2\,^1S_0$



# Electron/Proton Collisions

Inherently, electron/proton collisional excitation is a three (or more) body process, although this is not obvious at first glance:

$$e^- + I \rightarrow e^- + I^* \rightarrow e^- + I + \gamma$$

Of course, the ion I actually has at least 1 electron, and likely more. As a result, the atomic calculations of the cross section for these processes are non-trivial and subject to significant errors (30% is common).

# Electron/Proton Collisions

Usually, the cross section is written as a dimensionless quantity called the "collision strength" (which is a function of energy, as well as lower energy level *i* and upper energy level *j*):

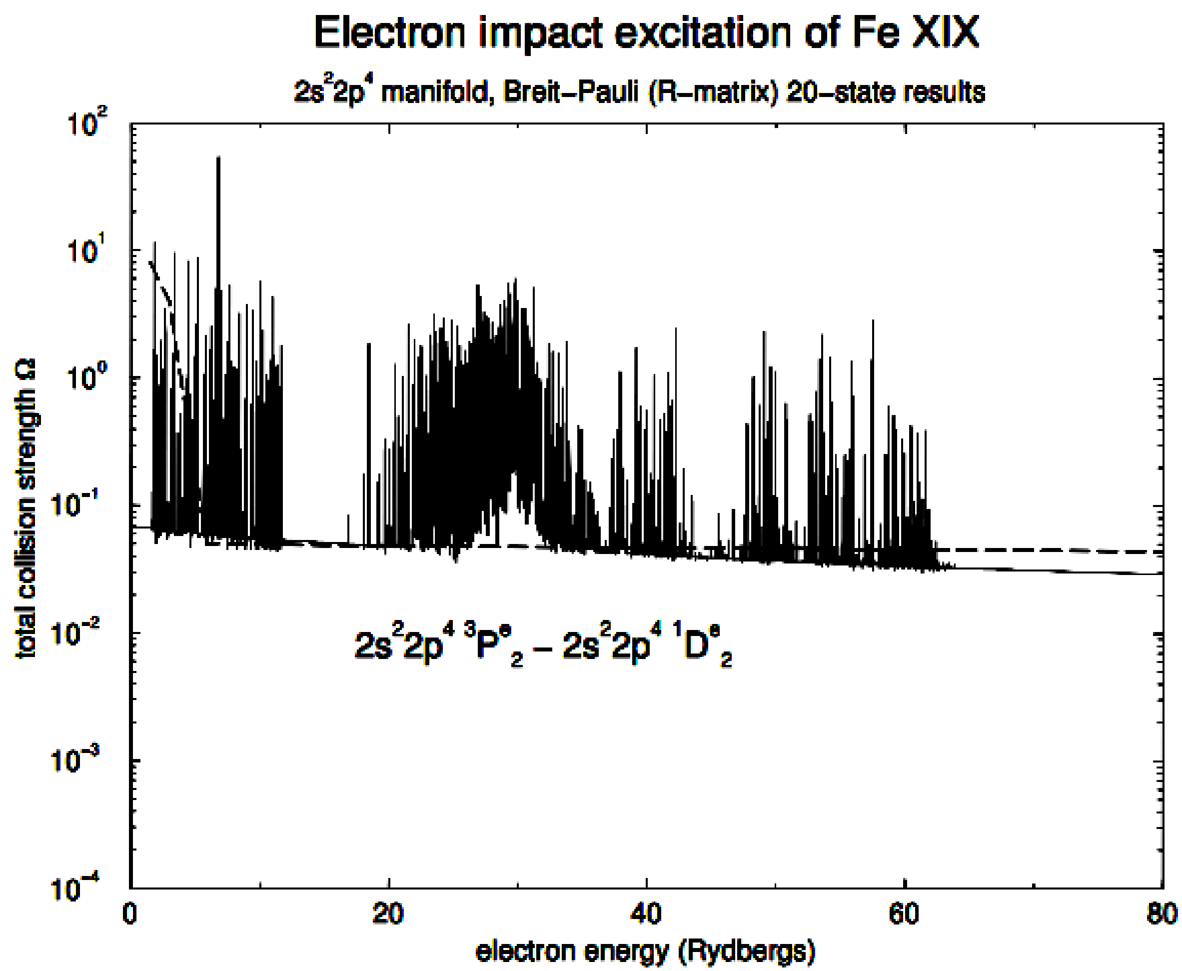
$$\Omega_{ij} = \frac{4\pi\omega_i}{\lambda^2} Q(i \rightarrow j)$$

This can be (and usually is) integrated assuming a Maxwellian velocity (*i.e.*, energy) distribution:

$$\Upsilon(T) = \int_0^\infty \Omega_{ij} \exp\left(-\frac{\Delta E_{ij}}{kT}\right) d\left(\frac{\Delta E_{ij}}{kT}\right)$$

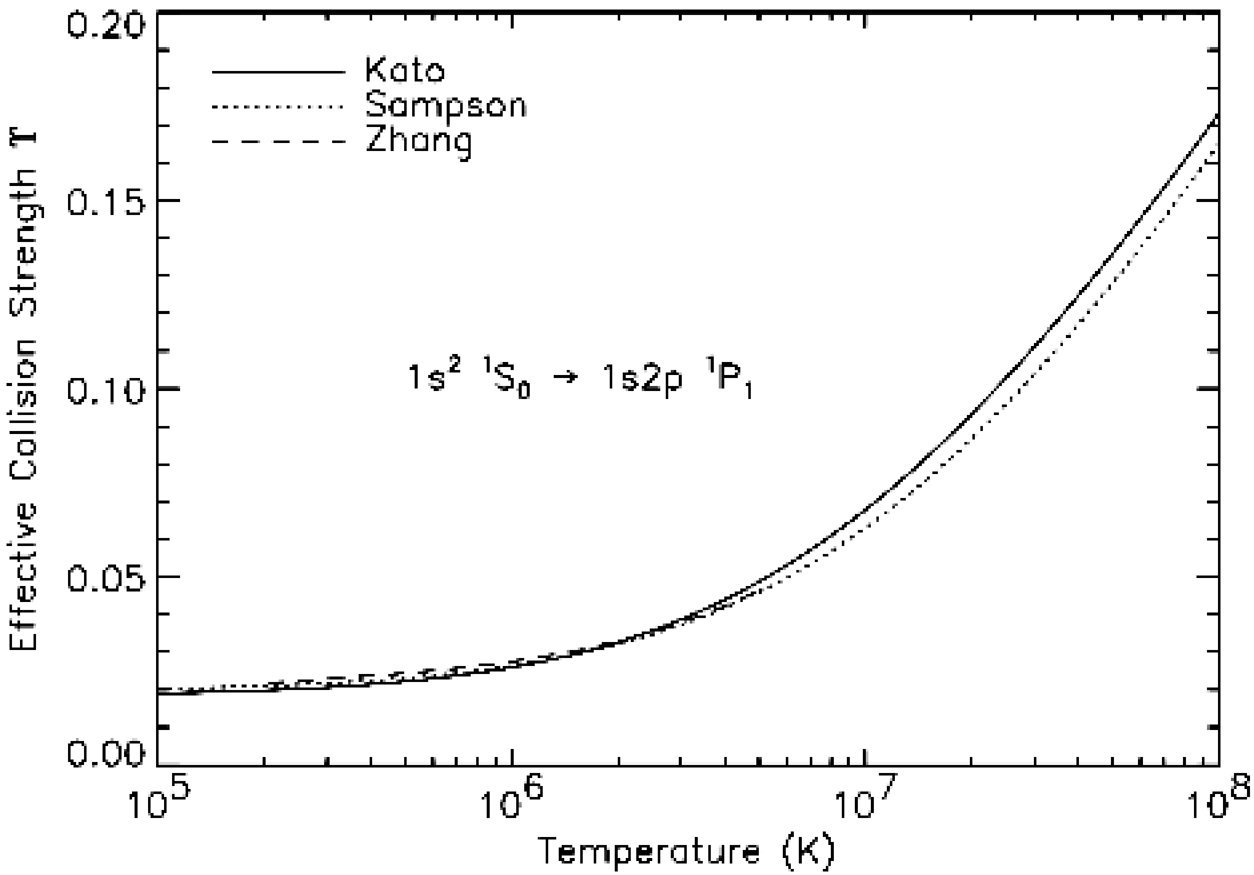
# Electron/Proton Collisions

Shown here is a calculated excitation collision strength for Fe XIX, using two different methods :



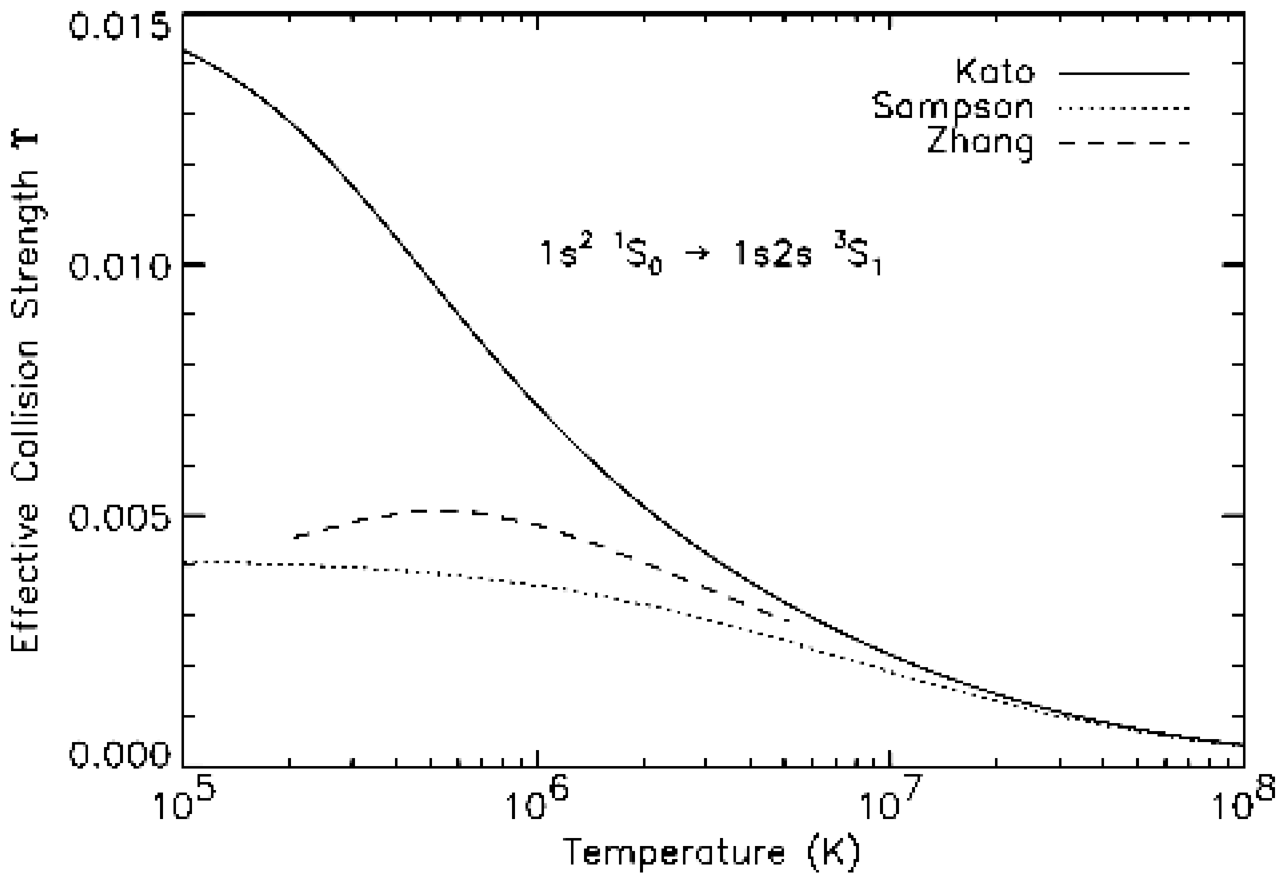
# Electron/Proton Collisions

Resonances such as those shown in the previous calculations may be significant or not, depending upon the "type" of transition. For resonance (allowed) transitions, ironically, resonances are not particularly important:



# Electron/Proton Collisions

Resonances (which occur near the transition energy, and thus are more important at lower temperatures) are more important for forbidden transitions:



# Electron/Proton Collisions

Just what **is** a resonance, in this terminology? It refers to a specific energy where the excitation cross section is enhanced. This is commonly due to some autoionizing level that is briefly populated by the colliding electron:

$$e^- + I \rightarrow I^{**} \rightarrow e^- + I^* \rightarrow I + \gamma$$

The electron excites the ion into a doubly-excited state, but then detaches itself before any further decay happens, leaving the ion in a singly-excited state. It is therefore a more important process for forbidden levels, where decay times are larger.

# Electron/Proton Collisions

Conveniently, there are some high-energy extrapolations for electron collisions. Burgess & Tully (1992) compiled these results:

- Electric Dipole: $\Omega(E \to \infty) = c \ln(E)$
- Multipole: $\Omega(E \to \infty) = c$
- Spin-change: $\Omega(E \to \infty) = c / E^2$

This particular feature of atomic physics has been used by the Chianti group in fitting collision strengths, guaranteeing proper extrapolations to high energy.

# Electron/Proton Collisions

And now for some words on Proton collisions.

In equilibrium, since protons are 1836× more massive than electrons, their speed will be ~43× slower than that of electrons. As a result, the collision rate $<n\sigma v>$ 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.

## Charge Exchange

Charge exchange is a process where an atom gives up an electron to a nearby ion, usually into an excited state.

In an astronomical context, the neutral ion is almost always hydrogen (helium is the only other real possibility), and that limits the importance of charge exchange to those regions where neutral hydrogen coexists with X-ray-emitting gas.

An example of such a region is the solar wind, which has plenty of highly ionized carbon and oxygen. This can charge exchange with neutral hydrogen in the solar system and lead to possibly significant emission. At low temperatures ($kT < 50$ eV) charge exchange may also significantly affect the ionization balance.

# Inner-shell Excitation

Electrons from an "inner" shell may be collisionally excited as well. In some cases this is unremarkable; in Fe XIX,

$$2s^2\,2p^4\,{}^3P_2 \rightarrow 2s\,2p^5\,{}^3P_0$$

could be called a innershell excitation. It decays with a 106.3Å photon but it isn't incredibly significant. However, some transitions are more important:

$$1s^2\,2s^1\,{}^2S_{1/2} \rightarrow 1s\,2s^2\,{}^2S_{1/2}$$

This excitation in Li-like ions creates a photon called the *q* line, which appears between the resonance and forbidden lines in the same ion's He-like system. Seeing this line shows that there is a noticeable amount of Li-like ion in the plasma.

## Radiative Recombination

Radiative recombination occurs when an electron collides with an ion and becomes bound, emitting a photon in the process:

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

Consider the energy balance in this interaction. Even if the electron has zero velocity, it has a certain binding energy $E_i$ in the $I^-$ ion. So the emitted photon has a minimum energy $E_i$, plus whatever energy the electron had to begin with.

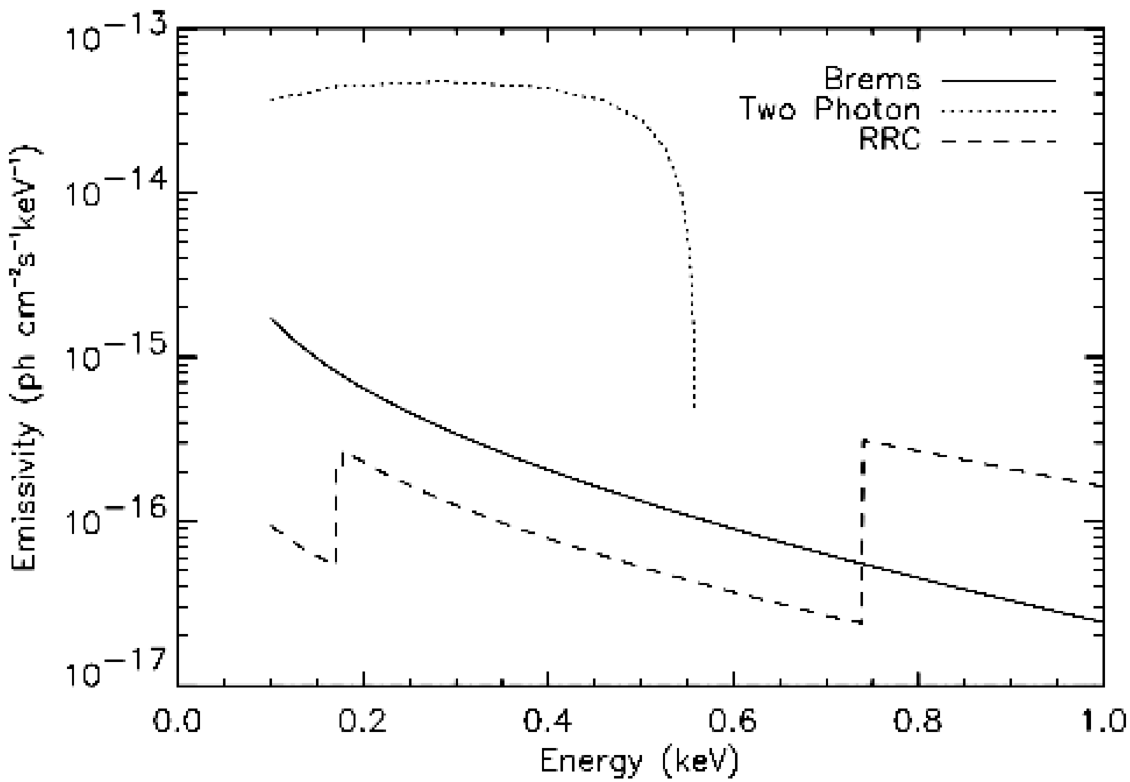
This process creates a continuum of emission, bounded at one end, called the Radiative Recombination Continuum (RRC).

# Radiative Recombination

In many cases the RRC is weak, but it is an excellent diagnostic if it can be measured.  The power emitted per keV is:

$$\frac{dE}{dt\,dV\,d\omega} = \frac{dP}{dE} = n_e n_{Z,j+1} E_\gamma \sigma^{rec}(E_e) v_e \frac{f(v)dv}{dE_\gamma}$$

Tucker & Gould 1966




Sample O VII (collisional) continuum

# Dielectronic Recombination

When an ion recombines dielectronically, two electrons are involved. The first electron recombines and is bound to the atom. Unlike RR, where the energy balance is maintained via an emitted photon, in DR a second electron is excited as well, putting the ion in a "doubly-excited" or "autoionizing" state.

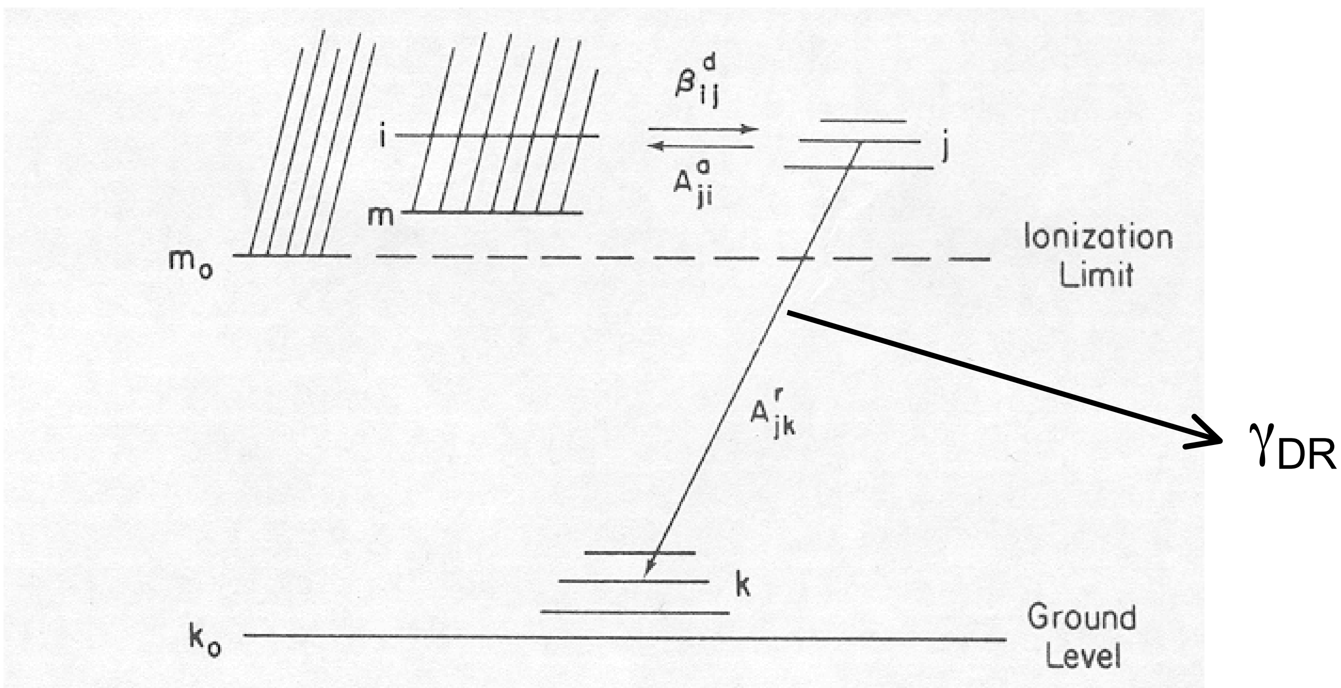
From there, it may ionize (resulting in either an elastic collision, or resonant excitation) or it may radiate, "relaxing" into a singly-excited state which then radiates as well.

Mathematically:

$$e^- + I \rightarrow I^{**} \rightarrow I^* + \gamma_{DR} \rightarrow I + \gamma$$

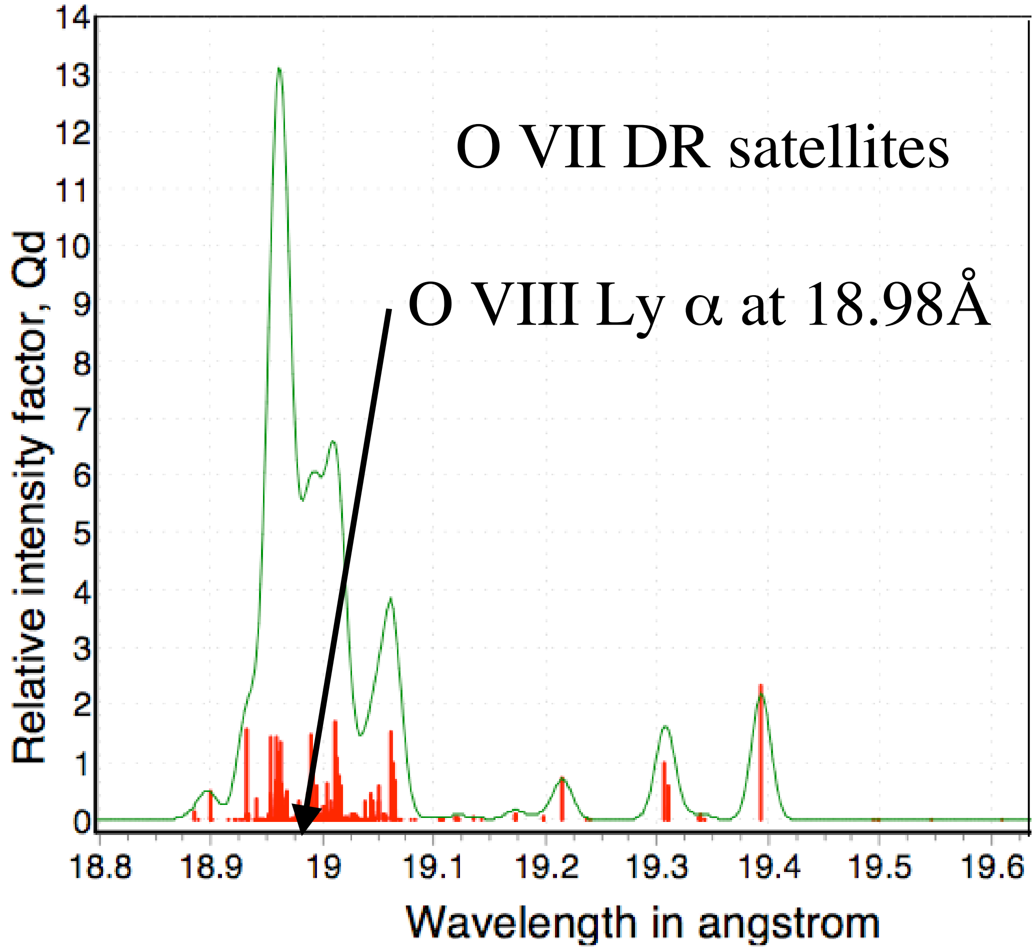
# Dielectronic Recombination

DR is a *resonant* process; the incoming electron must have an energy that matches that of the doubly-excited level, otherwise no transition will occur.



## Dielectronic Recombination

Photons emitted from the doubly-excited state are usually called "DR Satellite lines" because they are transitions made in the presence of an additional electron, so are shifted slightly to the red.



## Dielectronic Recombination

The dielectronic recombination rate for any given transition in a Maxwellian plasma is simply:

$$\text{Rate}_{DR} = n_I^+ \, n_e \, Q_d \exp(-E_{exc}/kT) \, /g_l$$

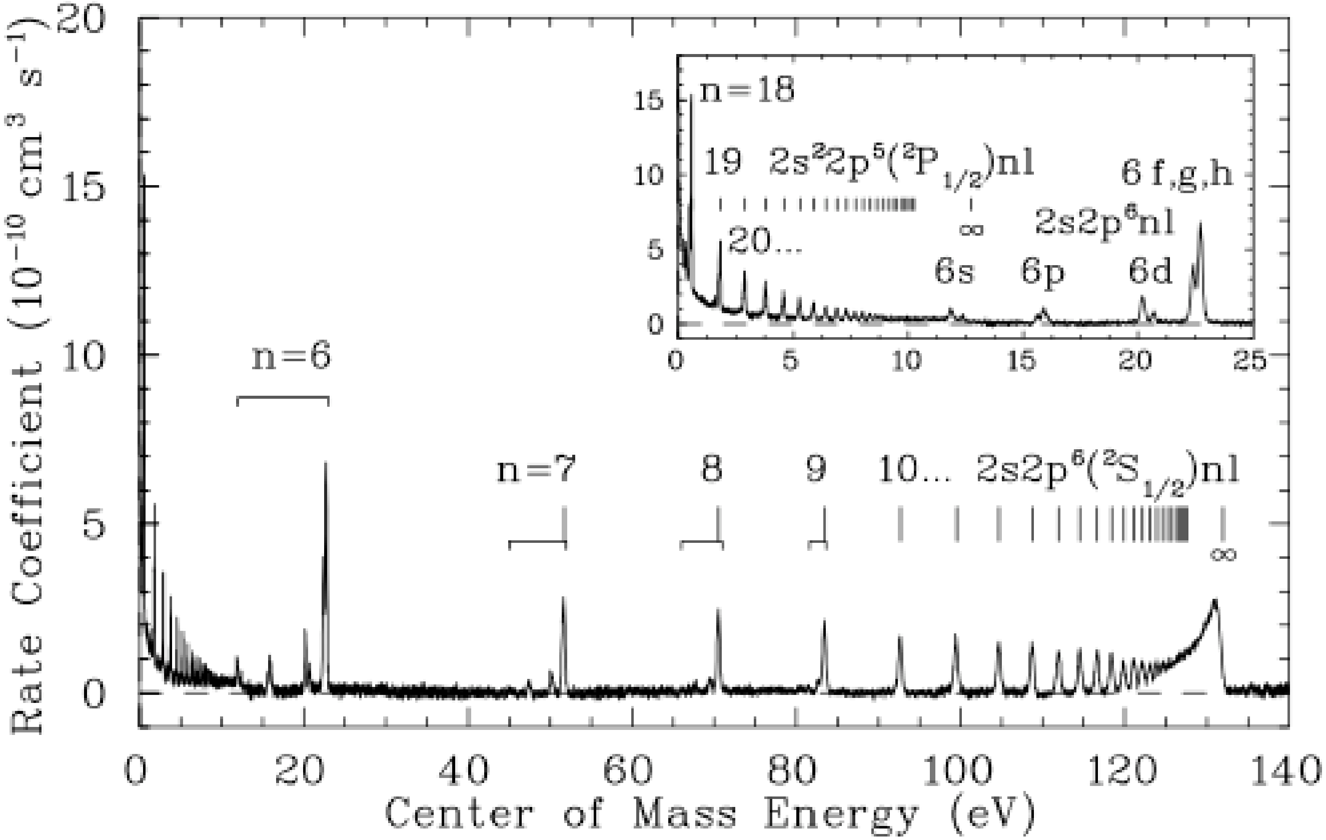
The two terms of note are $Q_d$, the total intensity, and $E_{exc}$, the excitation energy for the transition.

$\Delta n = 0$ DR transitions are those where the excited electron does not change principle quantum number *n*. As a result, its excitation energy will be very small.

$\Delta n = 1$ DR transitions are those where the excited electron does change principle quantum number *n*. As a result, its excitation energy will be large, on order the ionization energy.

# Dielectronic Recombination

A laboratory measurement of $\Delta n = 0$ DR on Fe XVIII (from Savin *et al*. 1999). Note the *resonances*, which are evident all the way down to 1 eV, despite the large ionization energy of Fe XVIII:



# Ionization

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

$$\text{Photoionization: } \gamma + I \rightarrow I^{+} + e^{-}$$

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

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

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

# Inner-shell ionization

Innershell ionization is more exciting. Usually in the X-ray regime, it refers to a K-shell (a/k/a 1s electron) being removed.

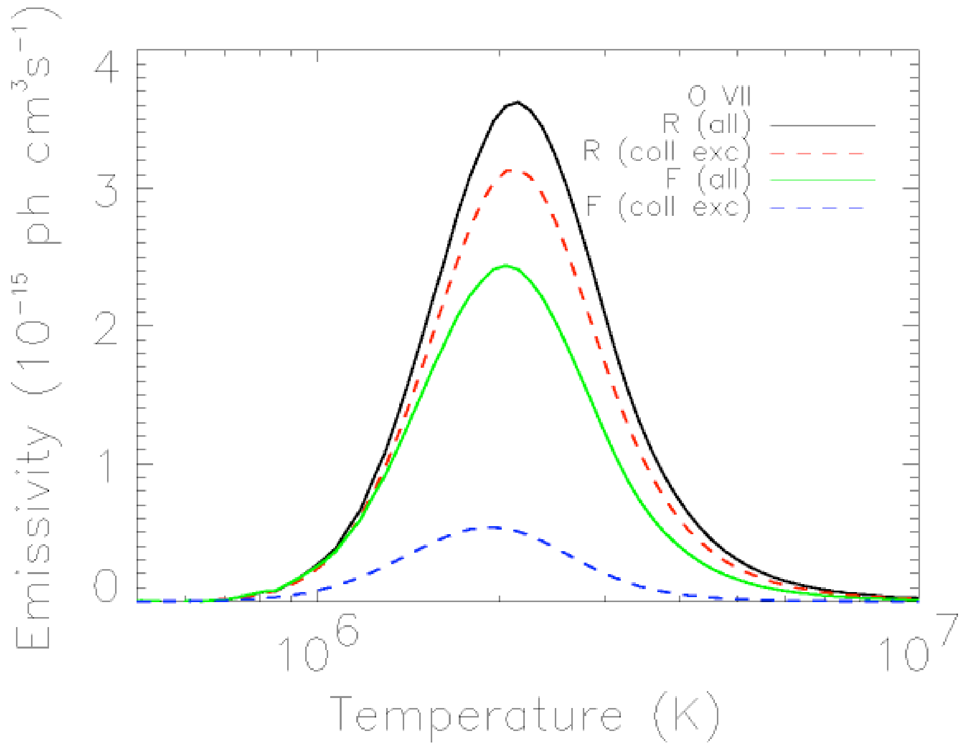
At this point, the ion is very unstable. It will either emit a photon (radiatively stabilize) or an electron, called an Auger electron. If the ion has be photoionized, this is also called a "photoelectron" and the number of electrons emitted the "photoelectric yield"

Whether a photon or an electron is emitted depends upon chance and the ion involved. As Z increases, the probability of a photon being emitted increases; for iron, it is ~30%. For oxygen, it is ~ 1%.

Innershell ionization of Fe I - Fe XVI tends to emit a 6.4 keV photon, commonly called the "cold" or "neutral" iron line.

# Error Estimates

This is much easier for some transitions than others. The resonance line of O VII (1s2p $^1P_1 \rightarrow 1s^2\ ^1S_0$) is dominated by collisional excitation:




But the forbidden line of O VII (1s2s $^3S_1 \rightarrow 1s^2\ ^1S_0$) is **not** dominated by collisional excitation.

# Basic Atomic Physics (for X-ray plasmas)

- Ionization (mostly easy)
  - Electron/Proton Collisions (i.e., “collisional plasma”)
  - Photoionization (i.e., “photoionized plasma”)
  - Innershell ionization (can emit photons)
- Recombination (harder)
  - Radiative (emits temperature-dependent continuum)
  - Dielectronic (dominates recombination; satellite lines)
  - Charge Exchange (comets; plasmas with neutral H)
- Excitation/De-excitation (harder)
  - Electron/Proton Collisions (resonances)
  - Photoexcitation (A values matter here)
  - Radiative Decay (emits observable photons!)

# Energy Levels

Groatrian diagram for
He-like Fe XXV

Some points to notice:

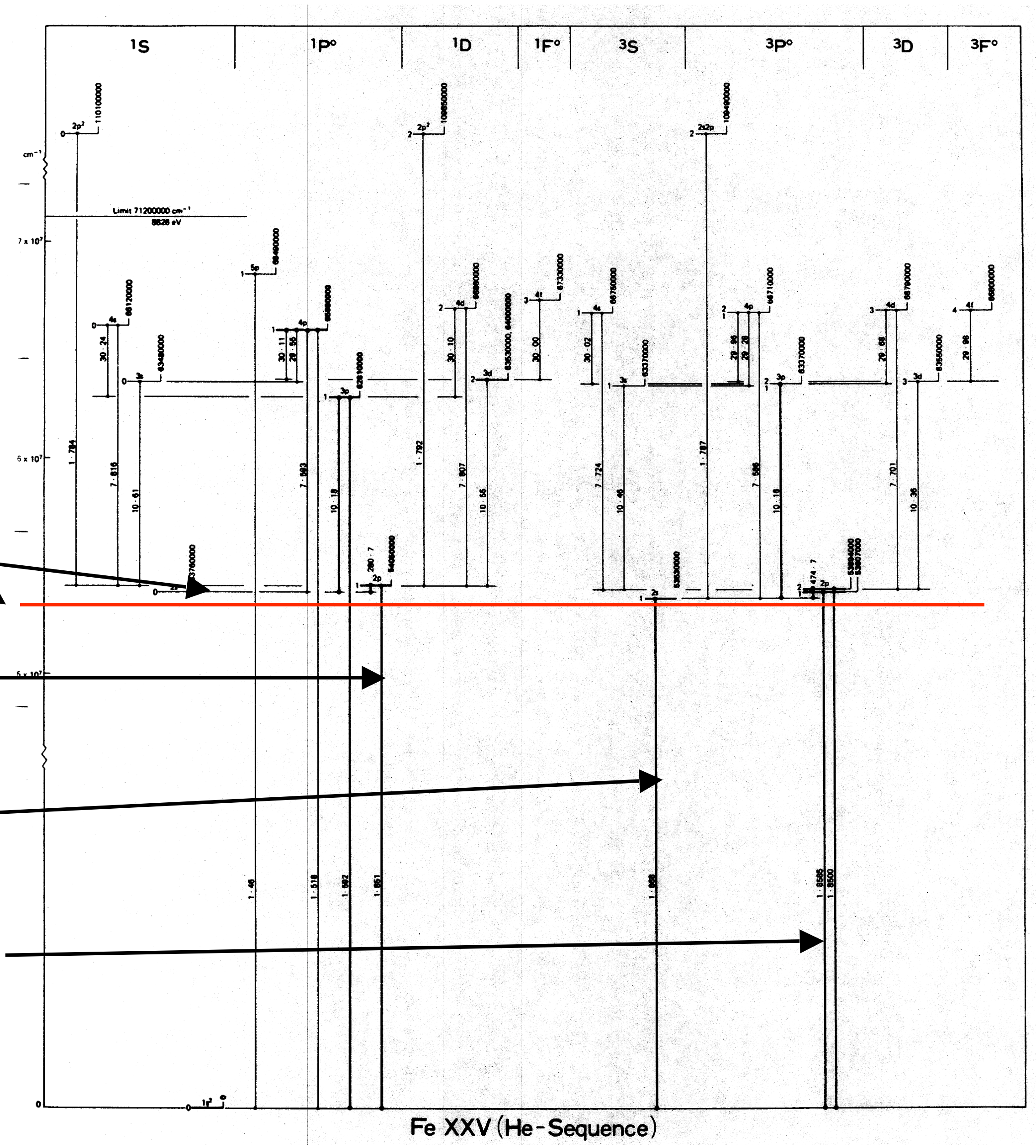
n = 2 level

Two-photon

Resonance line

Forbidden line

Intercombination line(s)



# Energy Levels

Of course, with more complex ions, the diagram becomes more complex.

In many cases, it is impossible to measure all of these levels in the lab. But the level energies (and thus wavelengths) can be inferred indirectly from other wavelengths.