Collisional Plasmas: A User's Guide

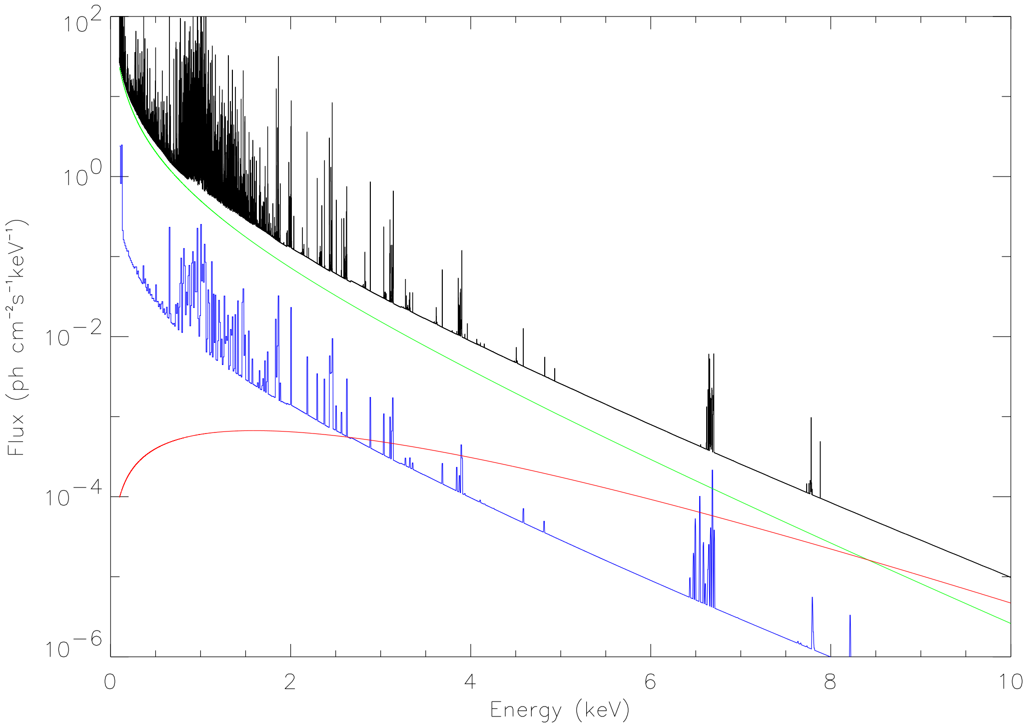
Randall Smith
Harvard-Smithsonian Center for Astrophysics

Sept 11, 2001

Collisional Plasmas

Topics to be covered:

- Comparision to other X-ray emission models
- CIE vs NEI: The Ionization Balance
- Atomic processes involved
- Physics of each process
- Available atomic data (and errors on same)
- Existing codes for calculating collisional plasma emissivities



All plasmas at 1 keV, unabsorbed:

Black APEC calculation of CIE plasma with Mazzotta et al. ionization balance.

Blue Raymond-Smith calculation (divided by 100) of CIE plasma

Green Bremsstrahlung

Red Blackbody

Note that at high temperature, the APEC continuum calculation exceeds the bremsstrahlung, due to the extra radiative recombination continuum.

The total emissivity in the APEC and Raymond-Smith calculations is similar; the differences are in the number of lines included and their wavelenths.

Thermal Plasmas Types

CIE : Collisional Ionization Equilibrium

Also known as:

- Raymond-Smith
- Mekal
- optically-thin thermal plasma

NEI : Non-Equilibrium Ionization

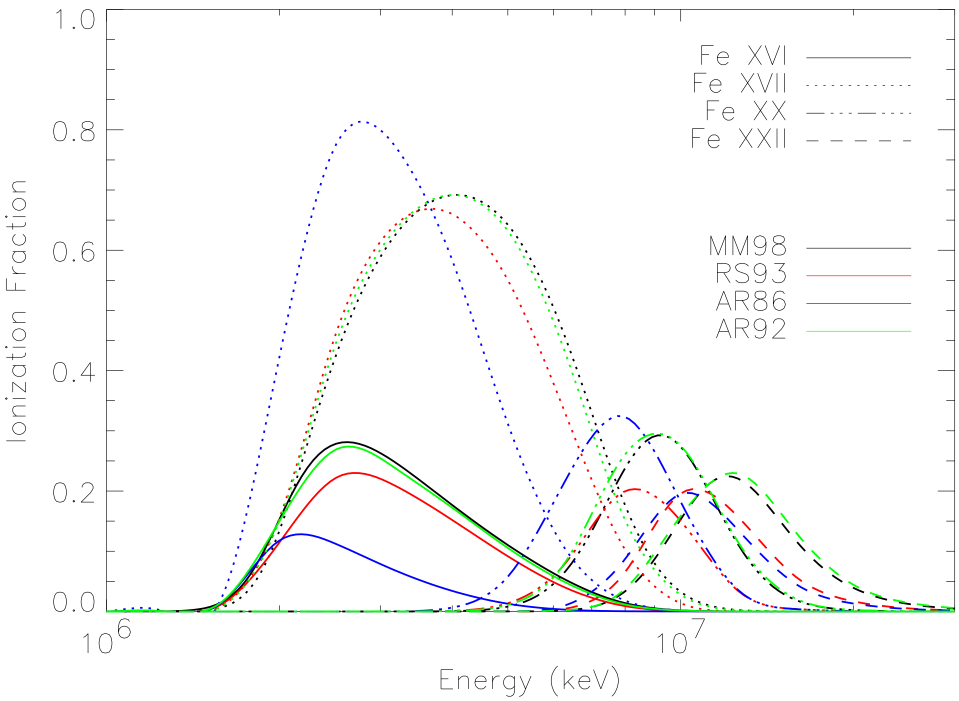
Also known as:

- Ionizing plasma
- Recombining plasma
- Thermal plus High-energy electron tail
- “Non-elephant biology”

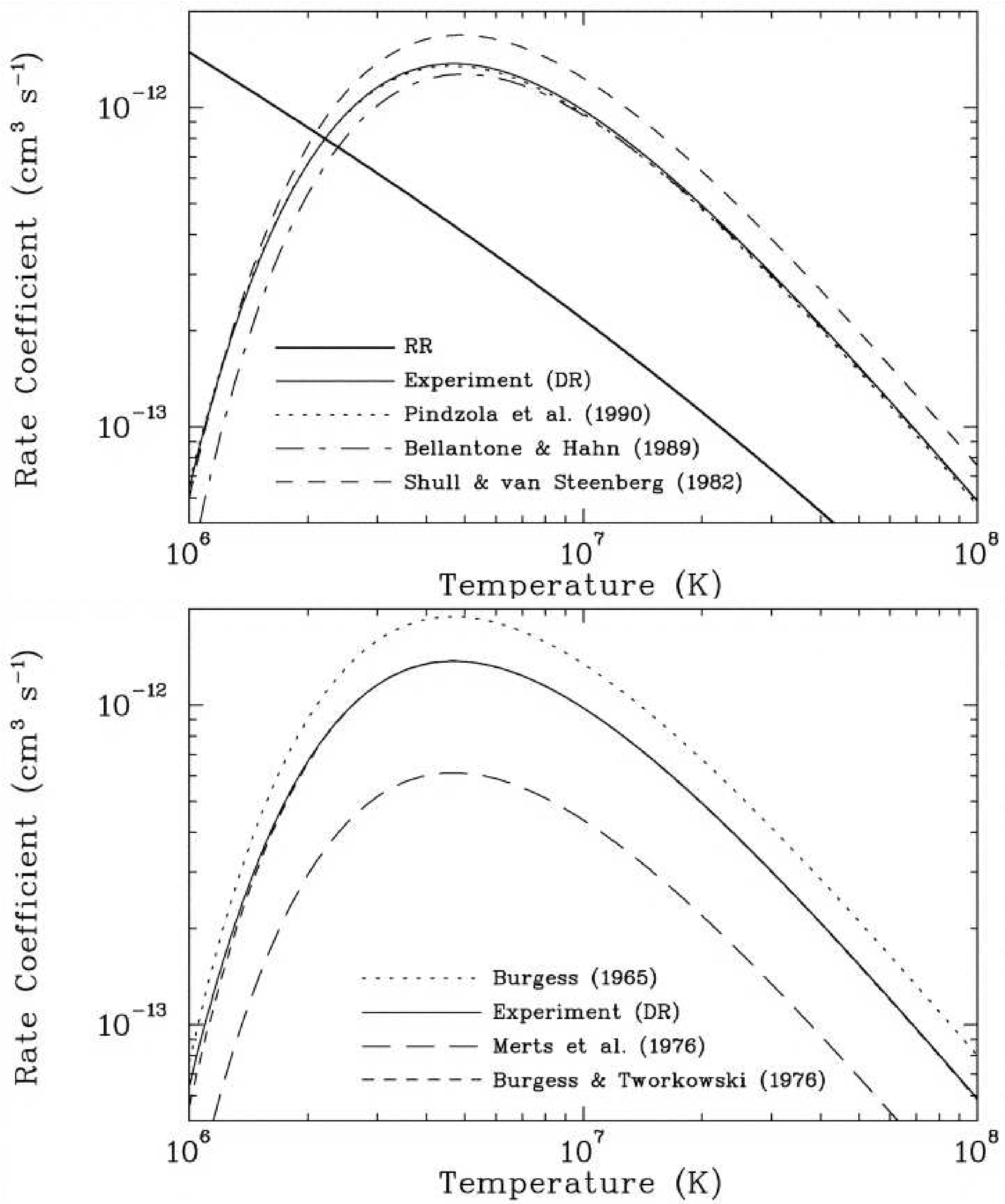
The ionization balance (in thermal equilibrium) depends on the rates for each ion:

- Total collisional ionization
- Excitation-autoionization
- Total radiative recombination
- Total dielectronic recombination

Of course, these are not known precisely. The plot compares three difference ionization equilibrium calculations: Arnaud & Rothenflug (1989), Raymond & Smith (1977; 1993 update), and Mazzotta et al. (1998). The ion fractions for Fe XVI, XVII, XX, and XXII are shown; the differences between modern calculations are in general between 1% and 10%, but can be substantially larger.

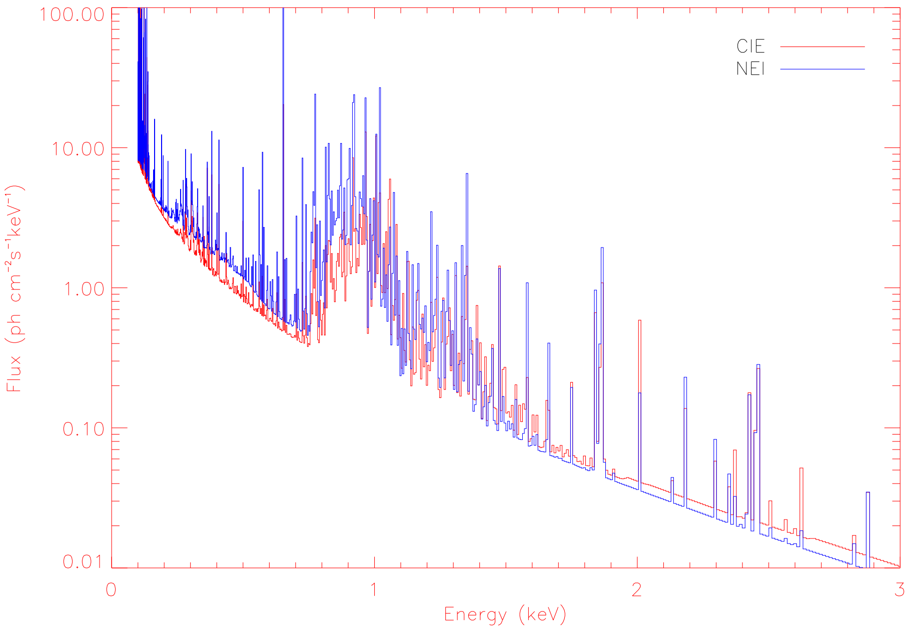


Various recombination rates for O VIII to O VII, via direct calculation (left) and using generic fitting formulae (right). (from Savin, 1999, ApJ, 523, 855)



Ionizing plasmas : $T_e > T_{ion}$

- Example is the plasma behind the shock front in a SNR
- innershell ionization and excitation-ionization play a major role.
- Strong forbidden line of Helium-like ions, due to ionization of $1s$ electron in $1s^2 2s$ system.
- Strong Fe K line at $\sim$ 6.4 keV, due to ionization of a $1s$ electron in Fe I-XXIV.



Recombining Plasmas : $T_e < T_{ion}$

- See talk on photoionized plasmas!

Physical Processes relevent to astrophysical plasmas:

- **Radiative Transitions** – Wavelengths, Einstein A coefficients
- **Electron Collisional Excitation** – $\Upsilon(T)$, the thermally-averaged excitation rate.
- **Proton Collisional Excitation** – Same for proton excitation, if significant.
- **Electron excitation-autoionization** – Rates to all relevent levels level
- **Dielectronic Recombination (Satellite Lines)** – Wavelengths and rates for each transition
- **Radiative Recombination (Continuum Emission)** – photoionization cross section for some levels
- **Two-Photon Continuum** – A-values, functional form of curve
- **Bremsstrahlung** – Relativistic vs Non.

In a CIE plasma, the ionization balance can be calculated independently of the level population. In an NEI plasma, all bets are off.

Note that we ignore:

- two-photon photoionization
- three-body interactions
- transitions involving molecules of all forms
- atom/atom collisions except with H II.

Issues to consider:

- Line identification
- Wavelengths (errors)
- A-values (checking for optically thick)
- LS vs jj coupling, issues involved

λ(Å)	Ion	Upper	Lower	Emissivity	kT	RelInt
13.4403	Fe XX	158	9	2.23e-18	0.862	0.005
13.4440	Fe XX	116	8	8.75e-18	0.862	0.022
13.4440	Fe XXII	17	8	2.24e-17	1.085	0.055
13.4473	Ne IX	7	1	4.06e-16	0.343	1.000
13.4510	Fe XVIII	67	1	1.23e-17	0.685	0.030
13.4550	Ne IX	10205	19	1.74e-18	0.273	0.004
13.4550	Ne IX	10206	20	3.12e-18	0.273	0.008

Ion Ne IX, energy level 1 —

electron configuration	:	$1s^2\ ^1S_0$
energy above ground (eV)	:	0.000000
Quantum state	:	n=1, l=N/A, s=0, degeneracy=1
Energy level data source	:	1983ADNDT..29..467S
Photoionization data source	:	1986ADNDT..34..415C

Ion Ne IX, energy level 7 —

electron configuration	:	$1s2p\ ^1P_1$
energy above ground (eV)	:	922.609985
Quantum state	:	n=2, l=1, s=0, degeneracy=3
Energy level data source	:	1983ADNDT..29..467S
Photoionization data source	:	1986ADNDT..34..415C

Ion Ne IX, 1 - 7 interactions —

Electron collision rate from 1 $\rightarrow$ 7	:	nonzero.
Reference bibcode	:	1983ADNDT..29..467S
Wavelength (lab/observed) (Angstrom)	:	13.447307 +/- 0.004000
Wavelength (theory) (Angstrom)	:	13.470000
Transition rate/Einstein A (s^{-1})	:	8.866670e+12
Wavelength (lab/observed) reference	:	1988CaJPh..66..586D
Wavelength (theory) reference	:	1983ADNDT..29..467S
Transition rate reference	:	1987JPhB...20.6457F

Electron Collisional Excitation

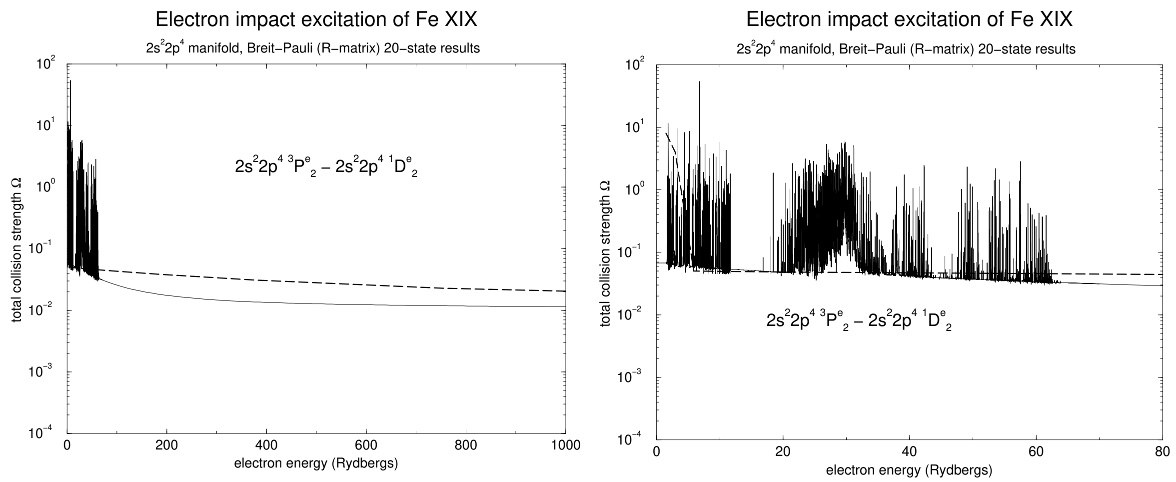
- Fundamental calculation is the cross section, which becomes a dimensionless quantity :

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

- Averaging this over a Maxwellian gives the "collision strength"

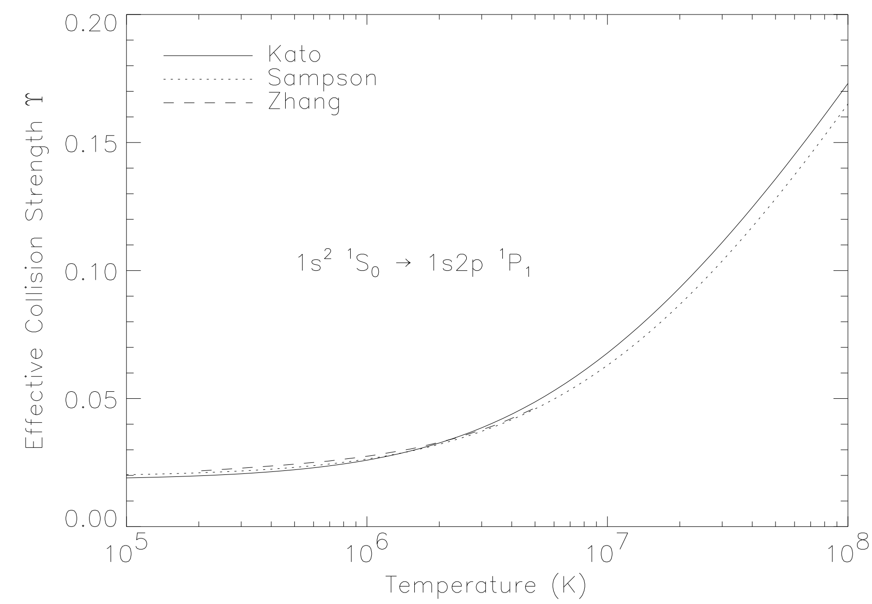
$$\Upsilon(T) = \int_0^\infty \Omega_{ij} \exp\left(-\frac{E_j}{kT}\right) d\left(\frac{E_j}{kT}\right)$$

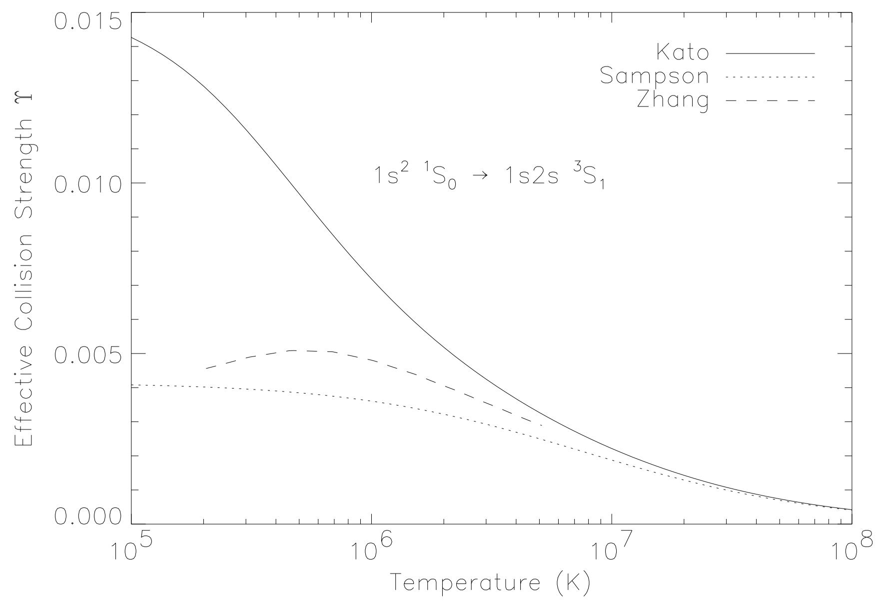
- High-temperature approximation (see Burgess & Tully 1992, A&A, 254, 436)
  - Electric dipole: $\Omega \to \text{const} \times ln(E)$
  - Multipole : $\Omega \to \text{const}$
  - Spin-change : $\Omega \to \text{const}/E^2$
- Threshold effects; R-MATRIX vs DW (from McLaughlin et al, 2001, J. Phys. B. in press)



Proton Collisional Excitation

- Similar notation
- In equilibrium, 1836× slower than electrons
- Affects mostly low-lying levels





The collison strength for the O VII $1s2p^1P_1 \to 1s^2\,{}^1S_0$ (R) line is not strongly affected by resonances. However, the same is not true for the forbidden transition, $1s2s^3S_1 \to 1s^2\,{}^1S_0$.

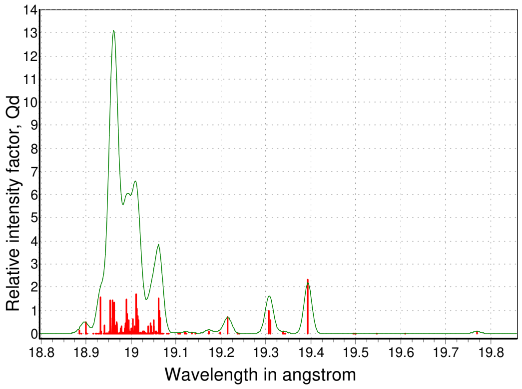
Consider O VIII in the ground state, recombining dielectronically. Thus we may have the following series of events:

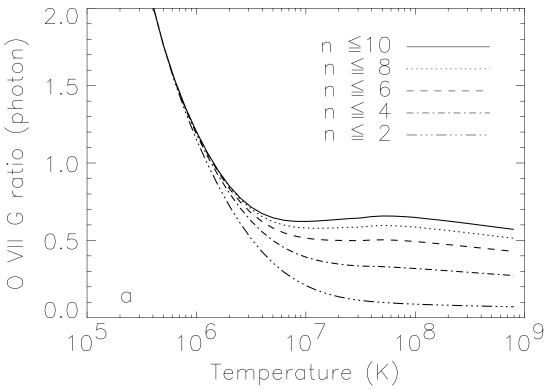
$$\begin{aligned} \text{O VIII } 1s^2S + e &\rightarrow \text{O VII } 2s3p^3P_2 \\ &\rightarrow \text{O VII } 1s2s^3S_1 + \gamma(16.485\text{Å}) \\ &\rightarrow \text{O VII } 1s^2\ {}^1S_0 + \gamma(22.10\text{Å}) \end{aligned}$$

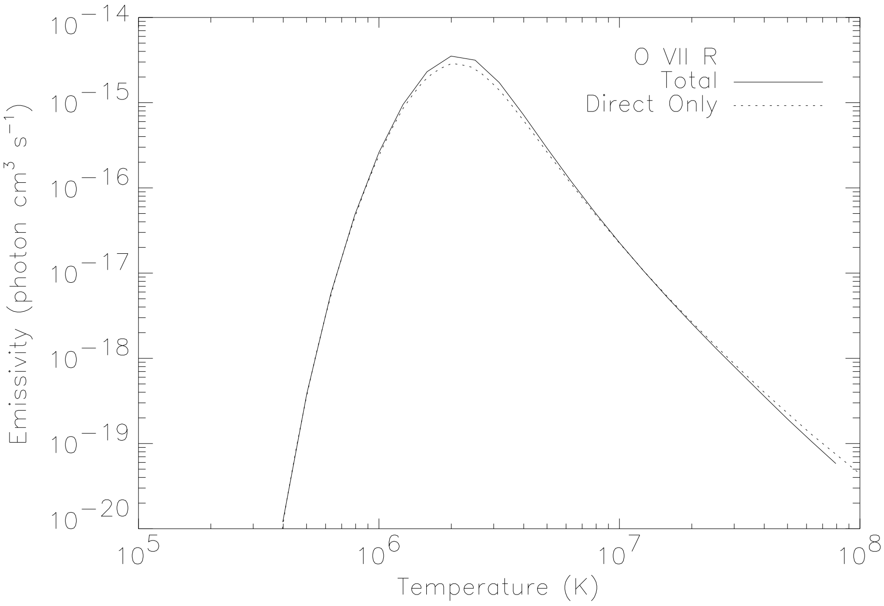
The inital "recombined" state is doubly-excited, which could:

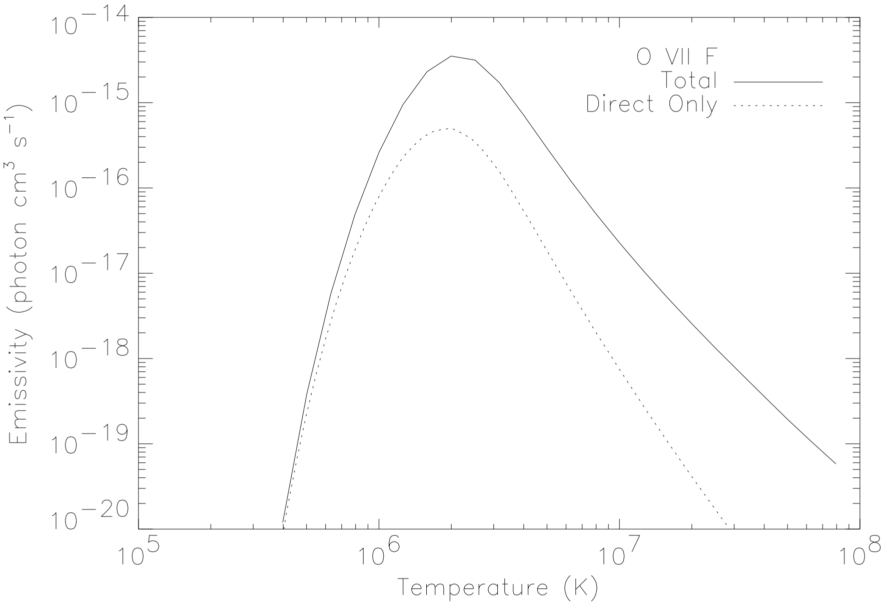
- Ionize and decay non-radiatively back to the ground state (elastic scattering)
- Ionize and decay to an excited state (resonant excitation).
- Radiatively stabilize, emitting at least 2 photons (dielectronic recombination)

Satellite lines, which occur in the presence of a spectator electron, may be slightly or significantly longer wavelengths than their main line, shown here for O VIII recombining to O VII (from Safronova et al. 2001, Can. J. Physics). In addition, dielectronic recombination can populate some levels significantly, in particular the forbidden line of O VII at high temperatures, when most of the line emissivity is from recombination (from Smith et al 2001 ApJ, 556, L91).









The emission due to direct excitation of a level is given by:

$$\epsilon(a \to b) = \frac{8.63 \times 10^{-6} \exp(-\frac{\Delta E}{kT})}{g_b \sqrt{T}} \Upsilon(a \to b) \frac{n_{\text{ion}}(T)}{n_Z} \times \frac{n_Z}{n_H} \tag{1}$$

Here, the emission of the resonance line is primarily due to direct excitation. However, the forbidden line is formed via secondary methods, such as recombination.

Radiative Recombination Continuum (RRC)

RRC occurs when an electron recombines radiatively ($I + e \rightarrow I^- + \gamma$) with an ion. The energy of the emitted photon is the kinetic energy of the electron plus the binding energy of the newly-recombined electron. Since the kinetic energy of the electron is not quantized, but the binding energy is a finite value, this forms a continuous spectrum with sharp edges at the binding energy of the levels. The power emitted per keV by this process is (Tucker & Gould 1966):

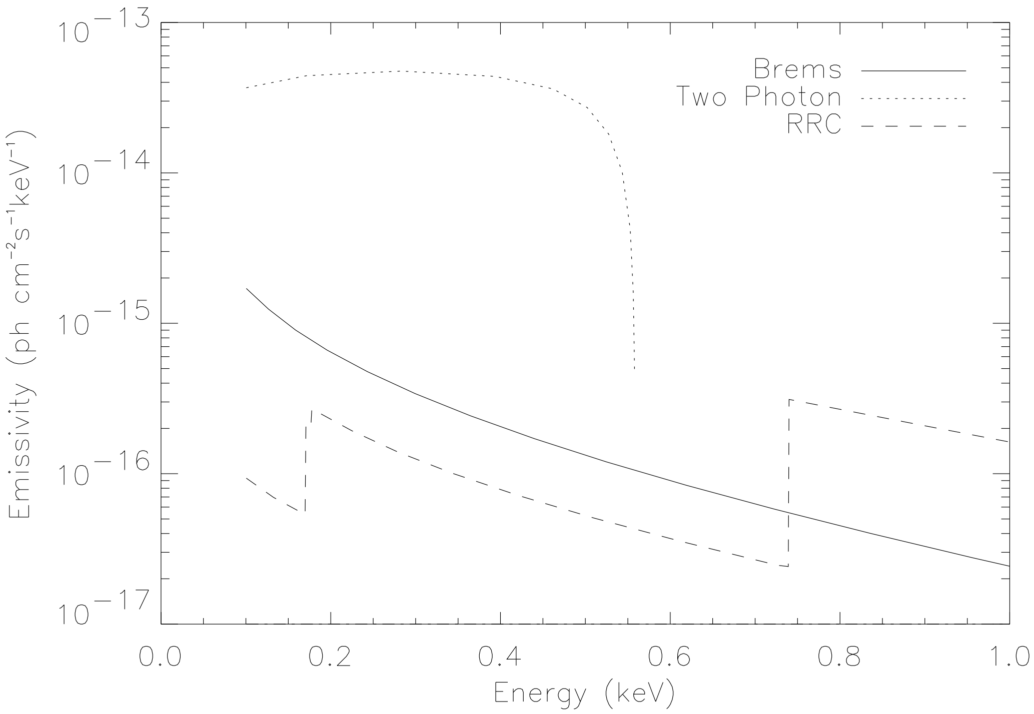
$$\frac{dE}{dtdVd\omega} = \frac{dP}{dE} = n_e n_{Z,j+1} E_\gamma \sigma^{rec}(E_e) v_e \frac{f(v)dv}{dE_\gamma} \tag{2}$$

Two-Photon Continuum

Two-photon transitions occur when a transition is absolutely forbidden, which occurs in hydrogenic ($2s^2S_{1/2} \rightarrow 1s^2S_{1/2}$) and helium-like ions ($1s2s^1S_0 \rightarrow 1s^{21}S_0$).

Bremsstrahlung

Will be covered in a future talk, and so is skipped here.

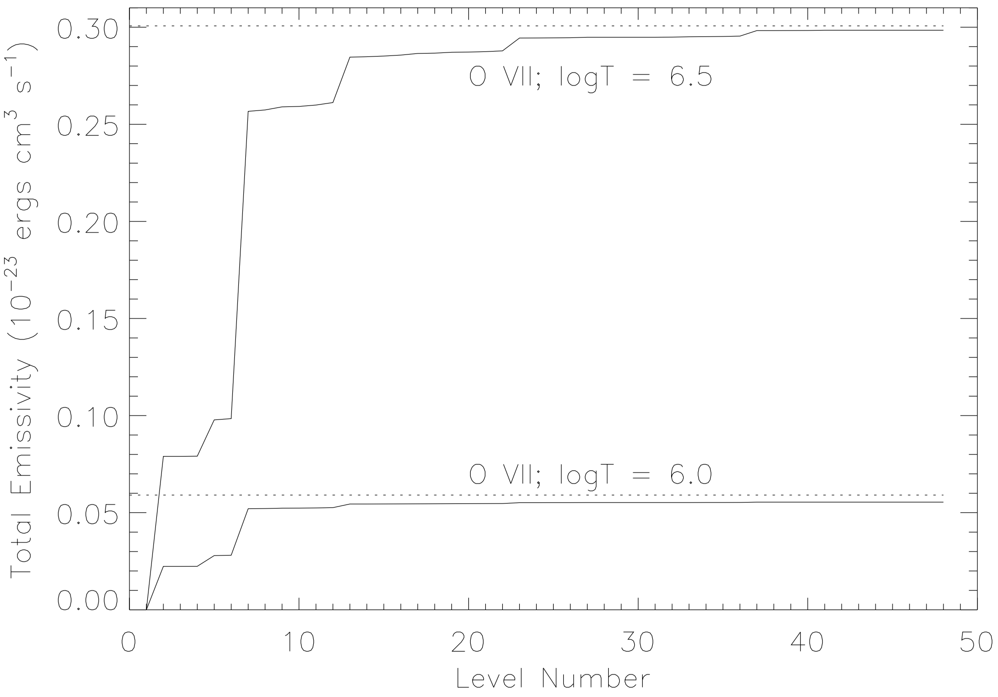


Doing error analysis with the underlying atomic data is far from trivial. However, it is far from impossible as well. Some suggestions are:

1. **Comparison of data** – Check different calculations. Although each plasma code chooses a standard "best" set for the emission tables, comparing different codes can be a measure of the errors. However, beware codes which appear different but are really using the same underlying data (for example, Sampson et al. on hydrogenic and helium-like ions)

2. **Sensitivity testing** – The "basic" error on much atomic collisional data is about 30%. In some cases, this may be irrelevant to your results, in others it will be the dominant error term. Explore the consequences of using the best rate $\pm 1\sigma$ for a particular ion or line parameter; if σ is not available, try using 30%.

3. **Monte Carlo modeling** – Although Monte Carlo assumes the errors on the data are uncorrelated, it's probably the best we have. Since theoretical atomic physics calculations tend to have systematic errors, each rate should be given a single offset and then calculated for a range of temperatures.



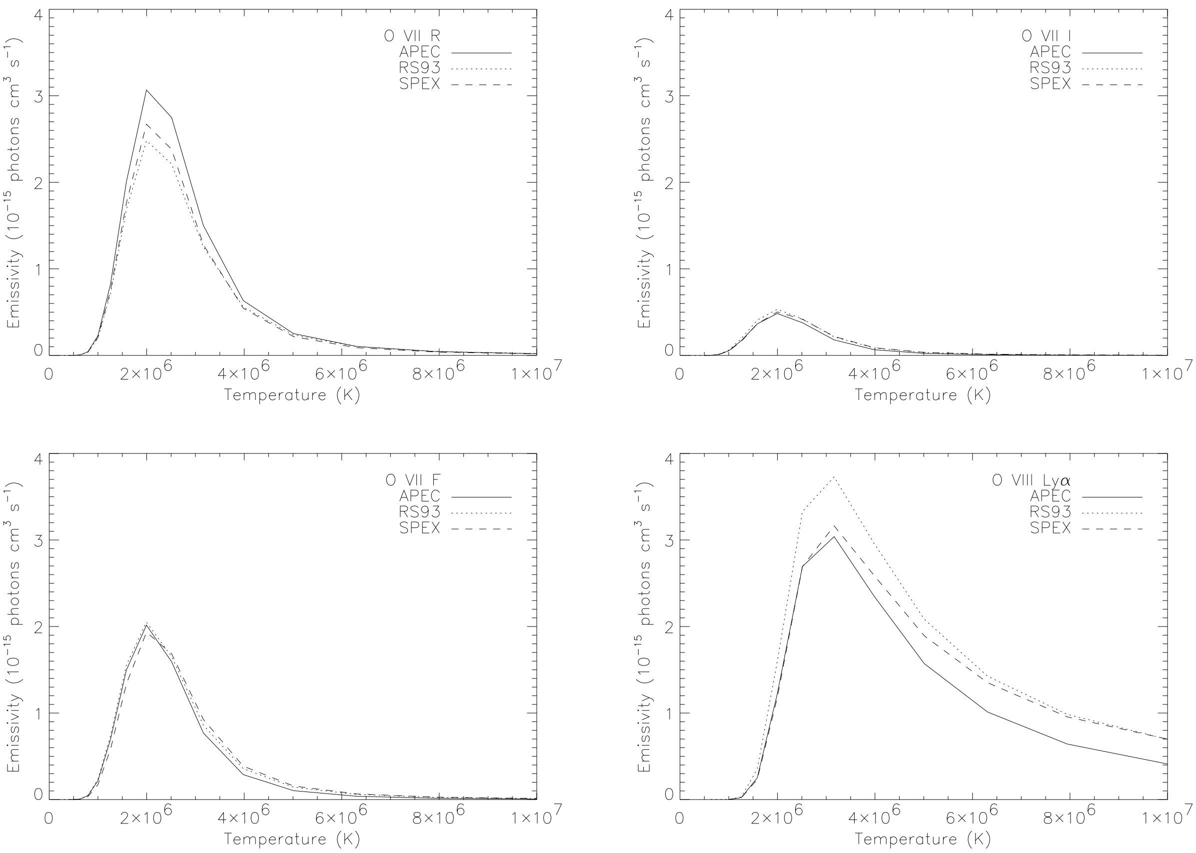
The total emissivity as a function of energy level, in O VII at 10^6 K and $10^{6.5}$ K. This shows that, in equilibrium, most of the emission comes from lower level states. The dotted lines show the total line emission, including emission from dielctronic satellite lines. Note that at the lower temperature, the relative DR contribution is larger.

I'm jumping into a specific data-file issue here, but it's hopefully going to be a standard, so I'm putting it in.

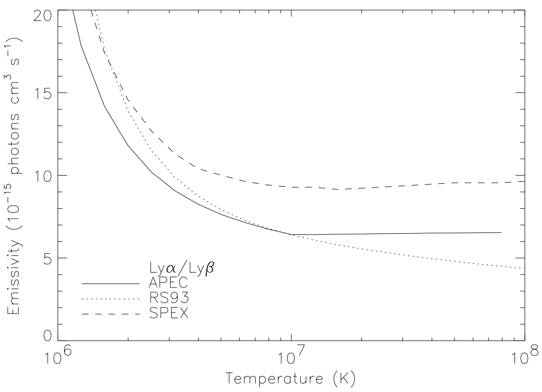
The plasma code APEC (http://hea-www.harvard.edu/APEC) has five different output formats:

- Line List: wavelengths, emissivities, and identities of the transition involved
- Continuum: summed emission from bremsstrahlung, two-photon, radiative recombination, and the "pseudo" continuum
- Complete Continuum: similar to the above, but separates each process by ion; to reduce table size, the spectrum is "linearly compressed"
- XSPEC Table Model: OGIP format FITS file, usable with the XSPEC "atable" command.
- New Table Model: Newly-defined format which will be used in upcoming versions of XSPEC and sherpa.

APEC outputs can easily become very large; the complete continuum files can be bigger than 500 MB.



Comparing the APEC, SPEX, and Raymond & Smith predictions for the O VII triplet and the O VIII Lyα line. Differences exist at the 10% level for some transitions.



Name	Source
Raymond-Smith	ftp://legacy.gsfc.nasa.gov/software/plasma_codes/raymond
SPEX	http://saturn.sron.nl/general/projects/spex
Chianti	http://wwwsolar.nrl.navy.mil/chianti.html
APEC/APED	http://hea-www.harvard.edu/APEC
HULLAC	Basic atomic physics code; not generally available
R-MATRIX	Basic atomic physics code; available on request

Biased Commentary

The **Raymond-Smith** code is fast, relatively small, and still quite accurate for CCD-resolution data. It includes both the ionization balance and the emissivity calculation. If you wish to incorporate thermal plasmas into a larger model, it is the code of choice.

The **SPEX** code does both CIE and a number of NEI models, but is available only as part of the SPEX analysis package, which is equivalent to XSPEC or Sherpa. It is the successor to the Mekal code, and contains much of the same data.

The **Chianti** code is heavily used by the solar community. It is written in IDL, and the code and data are completely separated, making it a good source of atomic data. It uses a tabulated ionization balance. Its strengths are in the optical/EUV, although they are working on including more X-ray lines.

The **APEC/APED** code is designed to be used to analyze high-resolution X-ray spectroscopy data from Chandra and XMM/Newton. The code and data are separate; all the input and output data are stored as FITS files. Currently, the ionization balance must be pre-calculated, but this limitation will be lifted soon.

The **HULLAC** code is a distorted-wave code which can handle ions with over 1000 levels. It is a general-purpose atomic physics code, and is not generally available. If a specific problem arises, however, a HULLAC user can generally be found who will do calculations.

The **R-MATRIX** code is a very specialized atomic physics code for doing collisional calculations. It is extremely difficult to use, but generally agreed to be the most accurate for calculations. However, at most a few 100 levels can be included.

Topics I hopefully covered:

- Comparision to other X-ray emission models
- CIE vs NEI: The Ionization Balance
- Atomic processes involved
- Physics of each process
- Available atomic data (and errors on same)
- Existing codes for calculating collisional plasma emissivities

- More work needs to be done on making the atomic data accessible. Moreover, we need closer collaborations with atomic physicists in order to get it done.
- Even *defining* what is meant by the error in the line emission model is not easy. However, there are a number of approaches (Monte Carlo, comparison of different calculations, Bethe approximation) that can be used in certain circumstances.
- Equilibrium calculations are much more likely to be accurate than non, since they can more easily be tested against lab data and they are the cases most carefully calculated by atomic physicists.
- When using line ratios as diagnostics, it is very important to understand what atomic data is being used
- Befriending atomic physicists is both useful (better understanding) and productive (they need help finding uses for their calculations)!