Atomic Lines:

Simple Ideas That Can Get Complicated

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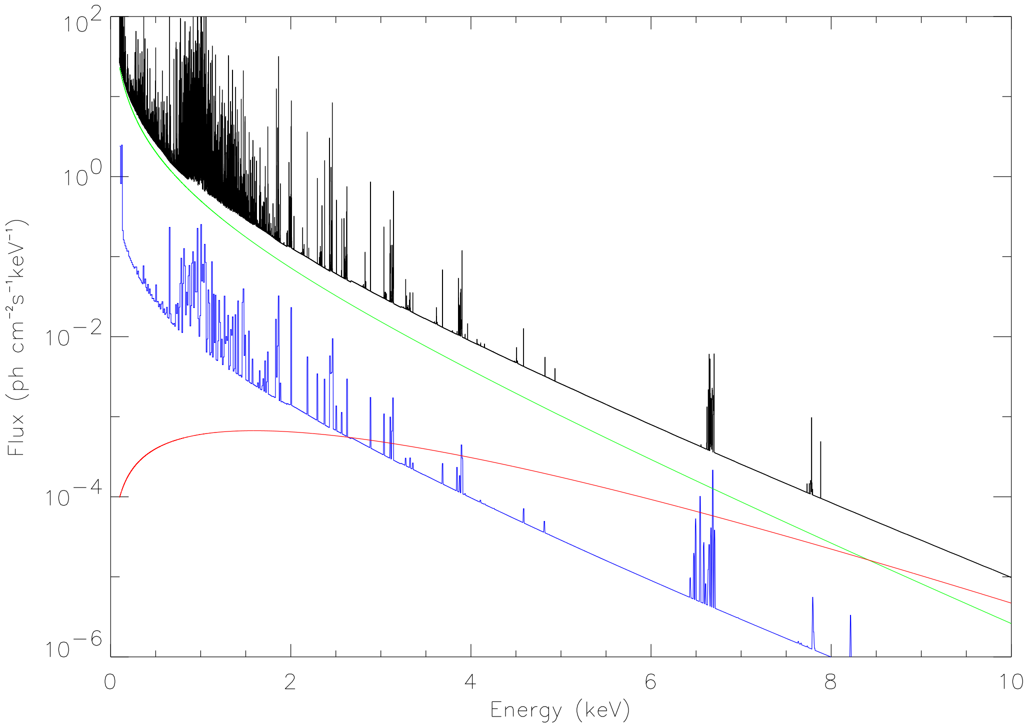
Topics I'm going to discuss:

- Basics of Emission Processes
- Merging Lab and Theory Data
- Emission codes for X-rays
- CIAO 2.2 and Emission Line Analysis
- Future X-ray Missions and Atomic Physics Needs

- Ice Cream Packing Technology



All plasmas at 1 keV, unabsorbed:

- APEC calculation of CIE plasma with Mazzotta et al. ionization balance.
- Raymond-Smith calculation (divided by 100) of CIE plasma
- Bremsstrahlung
- 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.

Electron Collisional Excitation

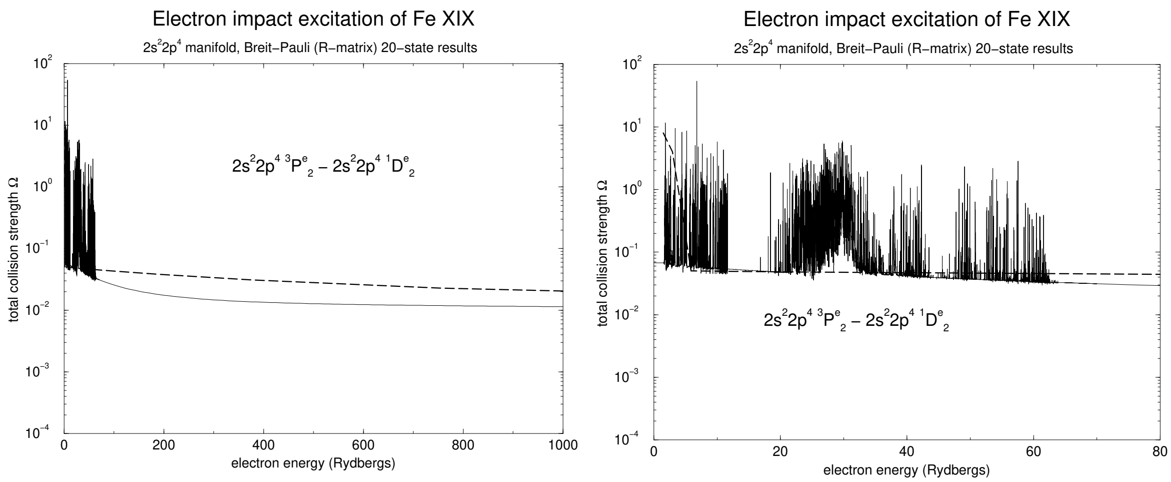
- Fundamental calculation is the cross section, which becomes a dimensionless quantity :

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

- 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: $\Omega \rightarrow \text{const} \times ln(E)$
  - Multipole : $\Omega \rightarrow \text{const}$
  - Spin-change : $\Omega \rightarrow \text{const}/E^2$
- 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

Dielectronic Satellite Lines

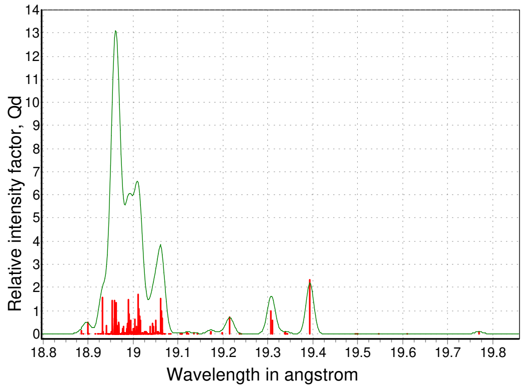
Consider O VIII in the ground state, recombining dielectronically. Thus we may have the following series of events:

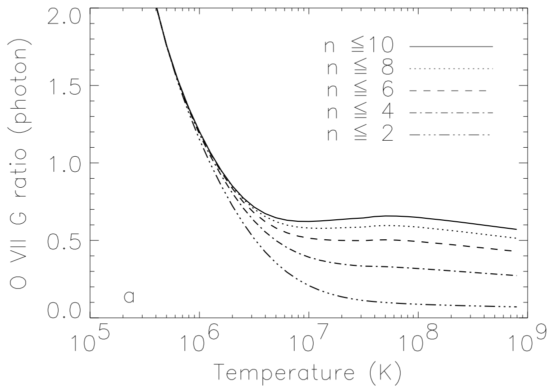
$$
\begin{aligned}
\text{O VIII } 1s\,^2\text{S} + e &\rightarrow \text{O VII } 2s3p\,^3\text{P}_2 \\
&\rightarrow \text{O VII } 1s2s\,^3\text{S}_1 + \gamma(16.485\text{Å}) \\
&\rightarrow \text{O VII } 1s^2\,^1\text{S}_0 + \gamma(22.10\text{Å})
\end{aligned}
$$

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).



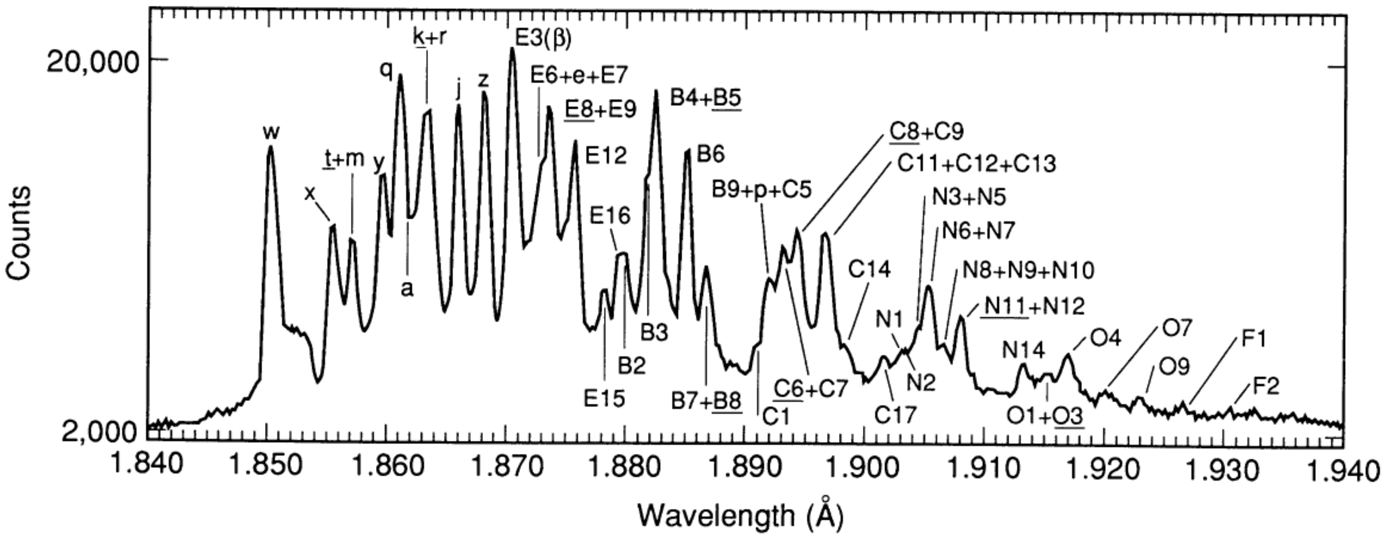


Innershell Excitation

Innershell/autoionizing emission lines are in some sense a more "general" category that includes dielectronic satellite lines. For example, the following are all ways to create an ion in an autoionizing state:

- Dielectronically recombine, creating two electrons in excited states
- Collisionally excite an innershell electron, for example the process O VI $1s^22s + e \to 1s2s2p \to 1s^22s + \gamma$
- Ionize an innershell electron, for example Fe XVII $1s^22s^22p^6{+}e/\gamma \to 1s2s^22p^6$, leaving the ion with a K-shell hole that is extremely unstable.

These transitions in iron, give rise to the famed "6.4 keV" (1.94Å) iron line. Excepting, of course, that that line is from neutral iron, and it is not a single line–it is in fact many lines. And higher ions of iron emit as well, as seen in this PLT tokamak spectrum (from Beiersdorfer et al. 1993)

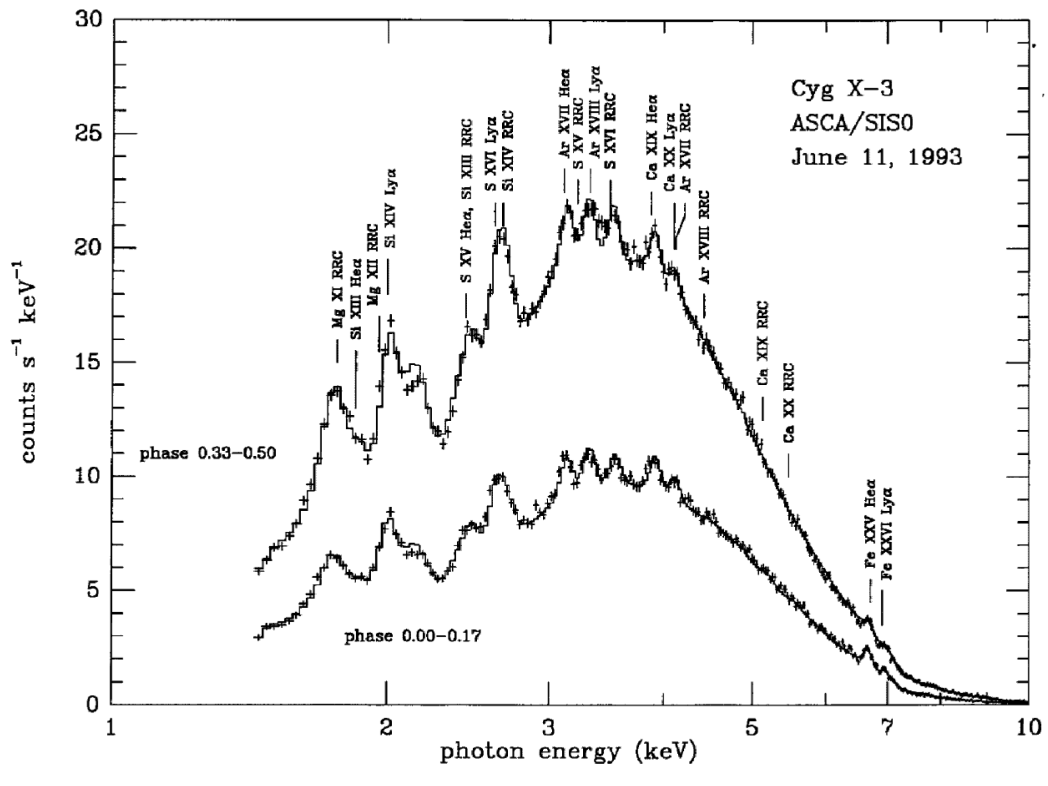


We are actively working to include these lines in the APED database; they are probably the primary "missing" component right now.

In a plasma whose electron temperature T_e is much less than the average ionization energy of the ions, the radiative recombination continuum is dominated by the ionization energy:

$$\frac{dP}{dE}(E_\gamma) = \frac{4\pi}{c^2}\frac{n_e n_{Z,j+1}}{(2\pi m_e kT)^{3/2}}E_\gamma^3\frac{g_{Z,j,n}}{g_{Z,j+1}}\exp(-\frac{E_\gamma - I_{Z,j,n}}{kT})\sigma^{ph}_{Z,j,n}(E_\gamma)$$

As a result, what in a high-temperature plasma is a broad feature appears as an oddly-shaped line in a photoionized plasma. This was seen in the ASCA SIS spectrum of Cyg X-3 (shown here from Liedahl & Paerels 1996):



And even if you're not interested in photoionized plasmas, the RRCs provide an excellent calibration, as there is almost no uncertainty in the underlying atomic physics.

Error Analysis with Atomic Data

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.

Measuring Wavelengths and Errors

In some cases, assigning wavelengths from laboratory measurements is simple, or even unnecessary. For example, hydrogenic lines wavelengths can be calculated with better precision than can be measured.
However, in other cases, matching lab data to theory calculations isn't so easy.

Wavelength-correcting Fe XVIII

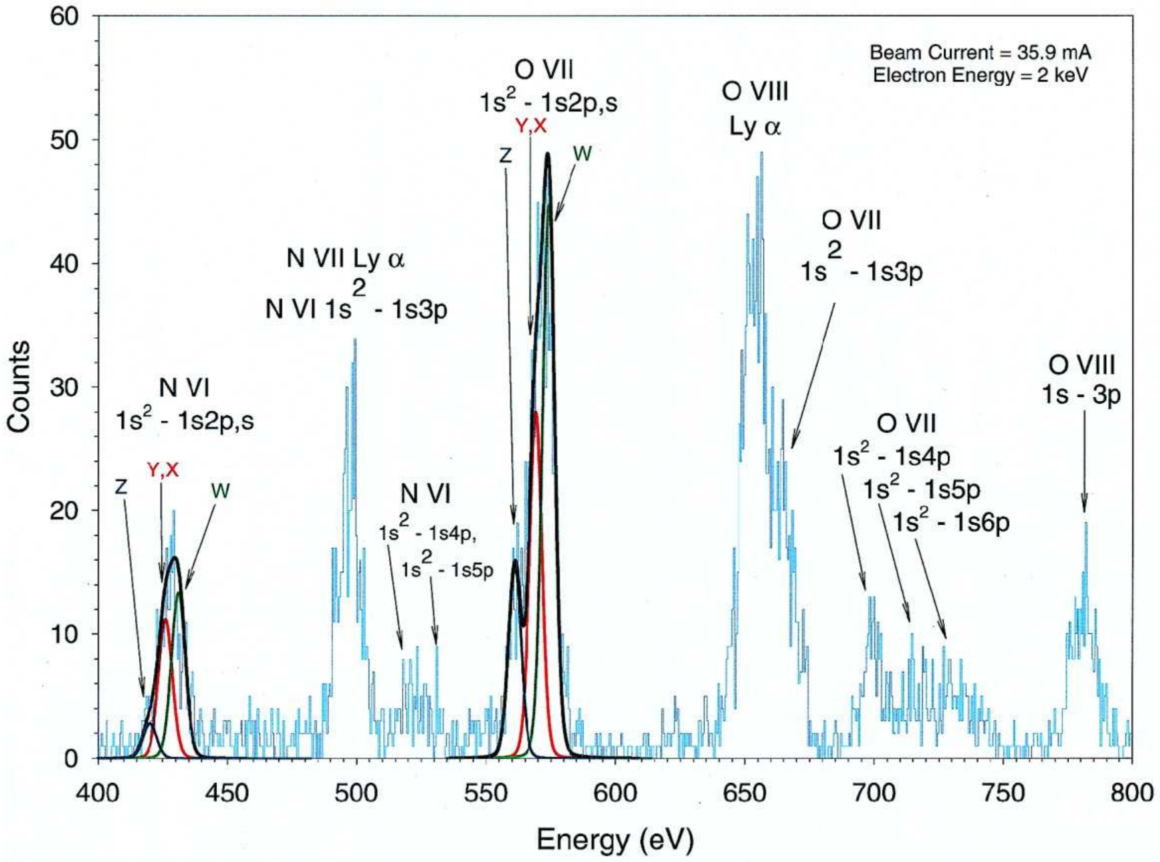
Begin with:

- HULLAC calculations up to $n = 6$: 501 levels (jj coupling), 13,095 radiative transitions
- Kelly data for about 70 levels (LS coupling)
- Lab data from the LLNL electron beam ion trap with a crystal spectrometer: 36 lines identified by wavelength and transition (jj coupling)
- Merge to create the following:

```
sherpa> describe(26,18,55,1)
Ion Fe XVIII, energy level 1 ---
electron configuration      : 2s^22p^5~^2P_{3/2}
energy above ground (eV)    : 0.000000
Quantum state               : n=2, l=1, s=N/A, degeneracy=4
Energy level data source    : 1997UNPUB.HULLAC..L
Photoionization data source : 1995A&AS..109..125V
-------------------------------------------
Ion Fe XVIII, energy level 55 ---
electron configuration      : 1s^22s^22p_{1/2}2p_{3/2}^33d_{5/2}
energy above ground (eV)    : 872.098877
Quantum state               : n=3, l=2, s=N/A, degeneracy=4
Energy level data source    : 1997UNPUB.HULLAC..L
Photoionization data source :
-------------------------------------------
Ion Fe XVIII, 1 - 55 interactions ---
Electron collision rate from    1 ->   55  : nonzero.
Reference bibcode                          : 1997UNPUB.HULLAC..L
Wavelength (lab/observed) (Angstrom)       : 14.208000 +/- 0.003000
Wavelength (theory) (Angstrom)             : 14.216900
Transition rate/Einstein A (s^-1)          : N/A
Wavelength (lab/observed) reference        : 1999LLNL.JC-136647B
Wavelength (theory) reference              : 1997UNPUB.HULLAC..L
Transition rate reference                  : 1997UNPUB.HULLAC..L
```

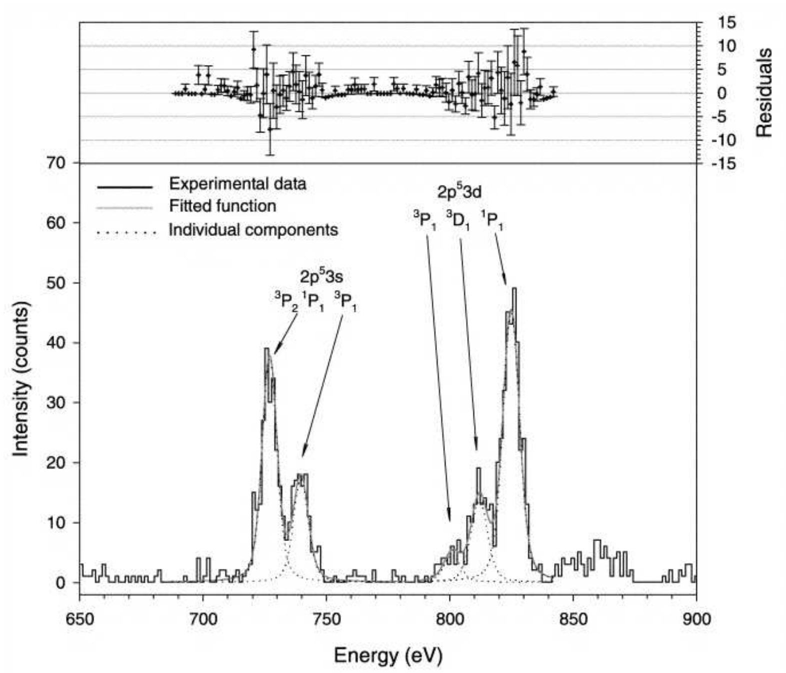
Measuring Line Ratios

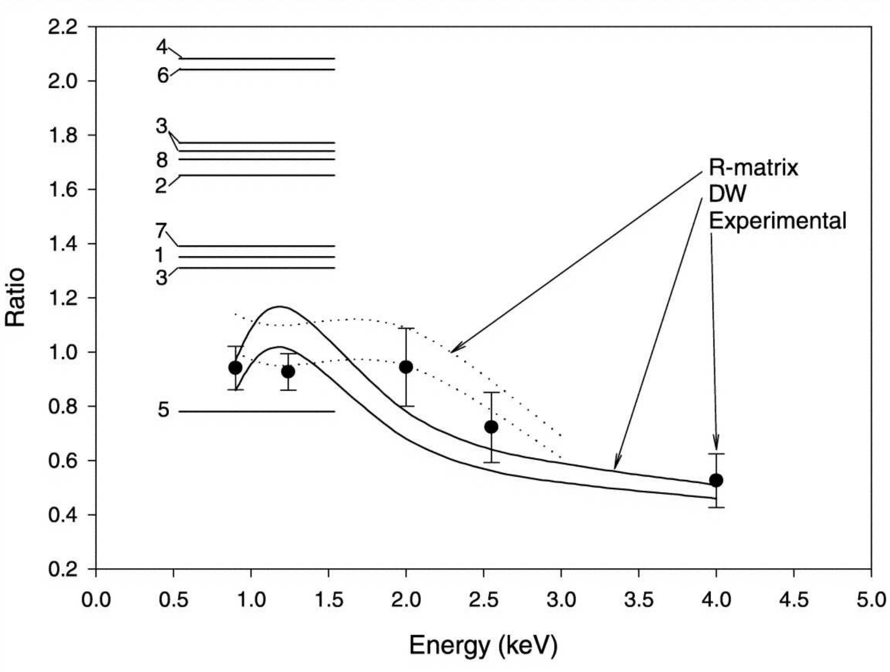
By using a microcalorimeter detector with an EBIT, broadband data can be taken very quickly, at a small loss of resolution compared to crystal spectrometers (from Silver et al 2000):



By taking a series of measurements at known density and electron energy, laboratory checks of well-known diagnostics can be made. Shown here is one such measurement from Laming et al. (2000) for the Fe XVII line ratio

$$\frac{2p^5 3s}{2p^5 3d} = \frac{I(16.780\AA) + I(17.055\AA) + I(17.100\AA)}{I(15.014\AA) + I(15.265\AA) + I(15.456\AA)}$$





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.

Available Photoionization Codes

Name	Source
XSTAR	http://heasarc.gsfc.nasa.gov/docs/software/xstar/xstar.html
Cloudy	http://www.pa.uky.edu/~gary/cloudy/
MAPPINGS III	http://www.mso.anu.edu.au/~ralph/index.html

Somewhat Less-Biased Commentary

The **XSTAR** code is the only code designed and built for the X-ray community. It was written by Tim Kallman, who actively maintains it with the aid of post-docs. It will output results in a format that can be used by XSPEC and Sherpa.

The **Cloudy** code is extremely well-documented, and is quite easy to use. It does include some X-ray lines now, but its main goal is to calculate optical and UV lines in photoionized plasmas accurately. Written by Gary Ferland, it is also well-maintained and nearing a new release.

The **MAPPINGS III** code by Ralph Sutherland is a general purpose astrophysical plasma modelling code. It is principally intended to predict emission line spectra of medium and low density plasmas subjected to different levels of photionization and ionization by shockwaves, from $10^2 - 10^8$ K.

Unlike collisional plasmas, photoionized plasmas must inherently include some model for the geometry of the source, making things that much more difficult. Optical depth effects are frequently important as well.

S-lang, Sherpa, and ISIS : Easy user-defined models

Using *S-lang*, we can create a new power-law model quite easily:

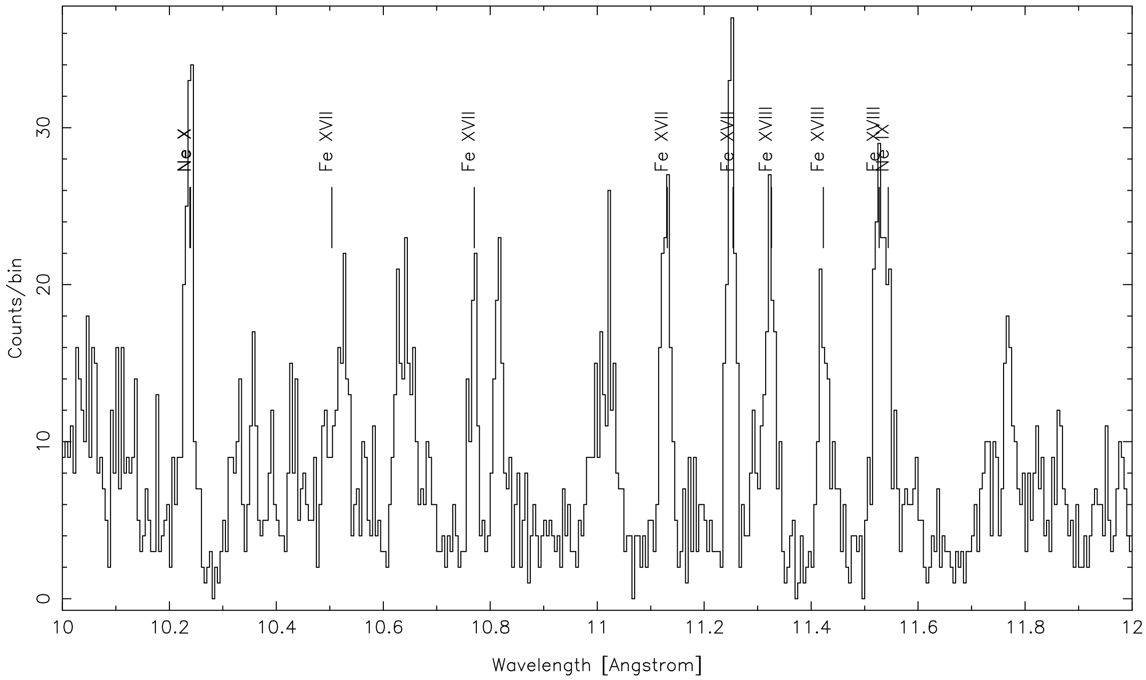
```
define powerlaw(p, norm, E, R) {

   variable Result = Float_Type [length(E)];
   variable dE = Float_Type [length(E)];

   for (i=1; i<length(E); i++) dE[i] = E[i] - E[i-1];
   Result = norm*(E^(-p))*dE;

   return Result;
}
() = sherpa_register_model("powerlaw",["power","norm"], 1,
    [1.0,1.e-2],   % default values
    [-10,1.e-20],  % Minimum values
    [10,1.e5],     % Maximum values
    [1,1]);        % Both thawed by default
```

The *ISIS* code can be run stand-alone, but as of CIAO 2.2, it can also be incorporated into Sherpa directly. Using a routine similar to the above, we can make thermal plasma models for any ion or set of ions, at any resolution we choose! We can then automatically identify the strong lines:



The new GUIDE command `identify` outputs line lists over a user-specified spectral range, along with an expected emissivity for each:

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

And of course more information on any given transition is available with the `describe` command:

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

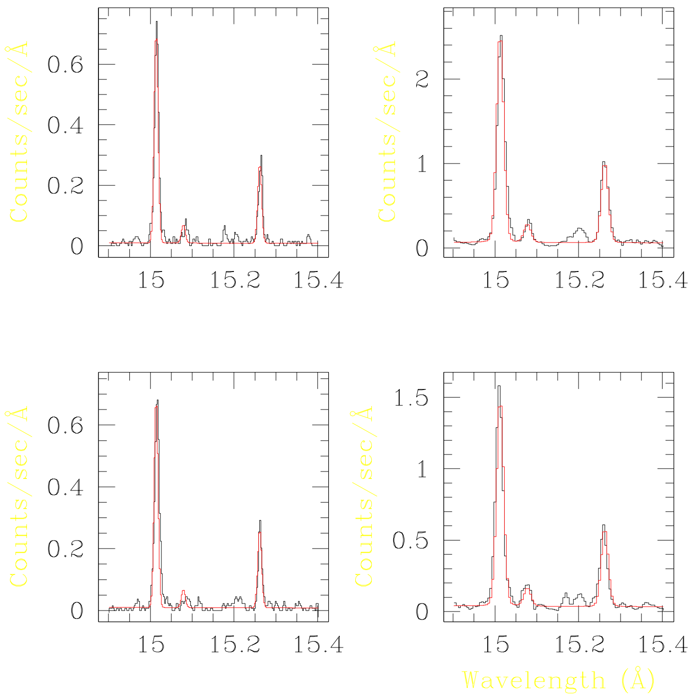
Given a “base” temperature, what lines should be strong?

```
sherpa> strong(1.e7,5.e-17,5,25)
The listed "Approximate Emissivity" is scaled from the peak value
using the ratio of the ionization balance at the requested temperature
and the peak temperature for the line.

                                    Approximate
  Lambda  --  Ion      UL -  LL Emissivity@   kT  RelInt  For More Info
 Angstrom                        ph cm^3/s   keV
   6.1804    Si XIV     4-   1  5.21e-17 @ 0.862 0.104 describe(14,14,4,1)
   6.6479   Si XIII     7-   1  8.77e-17 @ 0.862 0.175 describe(14,13,7,1)
   8.4192    Mg XII     4-   1  6.99e-17 @ 0.862 0.140 describe(12,12,4,1)
   9.4797    Fe XXI   248-   1  5.47e-17 @ 0.862 0.109 describe(26,21,248,1)
  11.7360  Fe XXIII    20-   5  8.39e-17 @ 0.862 0.168 describe(26,23,20,5)
  11.7700   Fe XXII    21-   1  1.94e-16 @ 0.862 0.388 describe(26,22,21,1)
  12.1321      Ne X     4-   1  9.14e-17 @ 0.862 0.183 describe(10,10,4,1)
  12.2840    Fe XXI    40-   1  5.01e-16 @ 0.862 1.000 describe(26,21,40,1)
  12.3930    Fe XXI    40-   2  9.01e-17 @ 0.862 0.180 describe(26,21,40,2)
  12.7540   Fe XXII    23-   6  7.17e-17 @ 0.862 0.143 describe(26,22,23,6)
  12.8220    Fe XXI    83-   7  6.62e-17 @ 0.862 0.132 describe(26,21,83,7)
  12.8240     Fe XX    60-   1  1.16e-16 @ 0.862 0.231 describe(26,20,60,1)
  12.8460     Fe XX    58-   1  2.83e-16 @ 0.862 0.565 describe(26,20,58,1)
  12.8640     Fe XX    56-   1  2.36e-16 @ 0.862 0.471 describe(26,20,56,1)
  12.9650     Fe XX    48-   1  8.77e-17 @ 0.862 0.175 describe(26,20,48,1)
  13.3850     Fe XX   111-   6  6.57e-17 @ 0.862 0.131 describe(26,20,111,6)
  13.4970    Fe XIX    71-   1  8.00e-17 @ 0.862 0.160 describe(26,19,71,1)
  13.5070    Fe XXI    42-   7  1.16e-16 @ 0.862 0.231 describe(26,21,42,7)
  13.5180    Fe XIX    68-   1  1.76e-16 @ 0.862 0.352 describe(26,19,68,1)
  13.7670     Fe XX    19-   1  5.56e-17 @ 0.862 0.111 describe(26,20,19,1)
  13.7950    Fe XIX    53-   1  7.07e-17 @ 0.862 0.141 describe(26,19,53,1)
  14.0080    Fe XXI    28-   7  9.31e-17 @ 0.862 0.186 describe(26,21,28,7)
  14.2080  Fe XVIII    55-   1  7.00e-17 @ 0.862 0.140 describe(26,18,55,1)
  14.2080  Fe XVIII    56-   1  1.28e-16 @ 0.862 0.256 describe(26,18,56,1)
  14.2670     Fe XX    54-   6  8.93e-17 @ 0.862 0.178 describe(26,20,54,6)
  14.3730  Fe XVIII    49-   1  5.04e-17 @ 0.862 0.101 describe(26,18,49,1)
  14.6640    Fe XIX    15-   1  5.34e-17 @ 0.862 0.107 describe(26,19,15,1)
  14.7540     Fe XX    33-   6  5.26e-17 @ 0.862 0.105 describe(26,20,33,6)
  15.0140   Fe XVII    27-   1  1.00e-16 @ 0.862 0.200 describe(26,17,27,1)
  15.0790    Fe XIX    11-   1  6.02e-17 @ 0.862 0.120 describe(26,19,11,1)
  16.0710  Fe XVIII     4-   1  5.85e-17 @ 0.862 0.117 describe(26,18,4,1)
  16.1100    Fe XIX    37-   6  7.83e-17 @ 0.862 0.156 describe(26,19,37,6)
  17.0510   Fe XVII     3-   1  5.54e-17 @ 0.862 0.111 describe(26,17,3,1)
  17.0960   Fe XVII     2-   1  5.27e-17 @ 0.862 0.105 describe(26,17,2,1)
  18.9671    O VIII     4-   1  1.22e-16 @ 0.862 0.244 describe(8,8,4,1)
  18.9725    O VIII     3-   1  5.88e-17 @ 0.862 0.118 describe(8,8,3,1)
```

After fitting a series of emission lines with Sherpa using the model:

```
source 3,4,8,9,10,11 = poly[b1]+delta1d[l1]+delta1d[l2]+delta1d[l3]
```



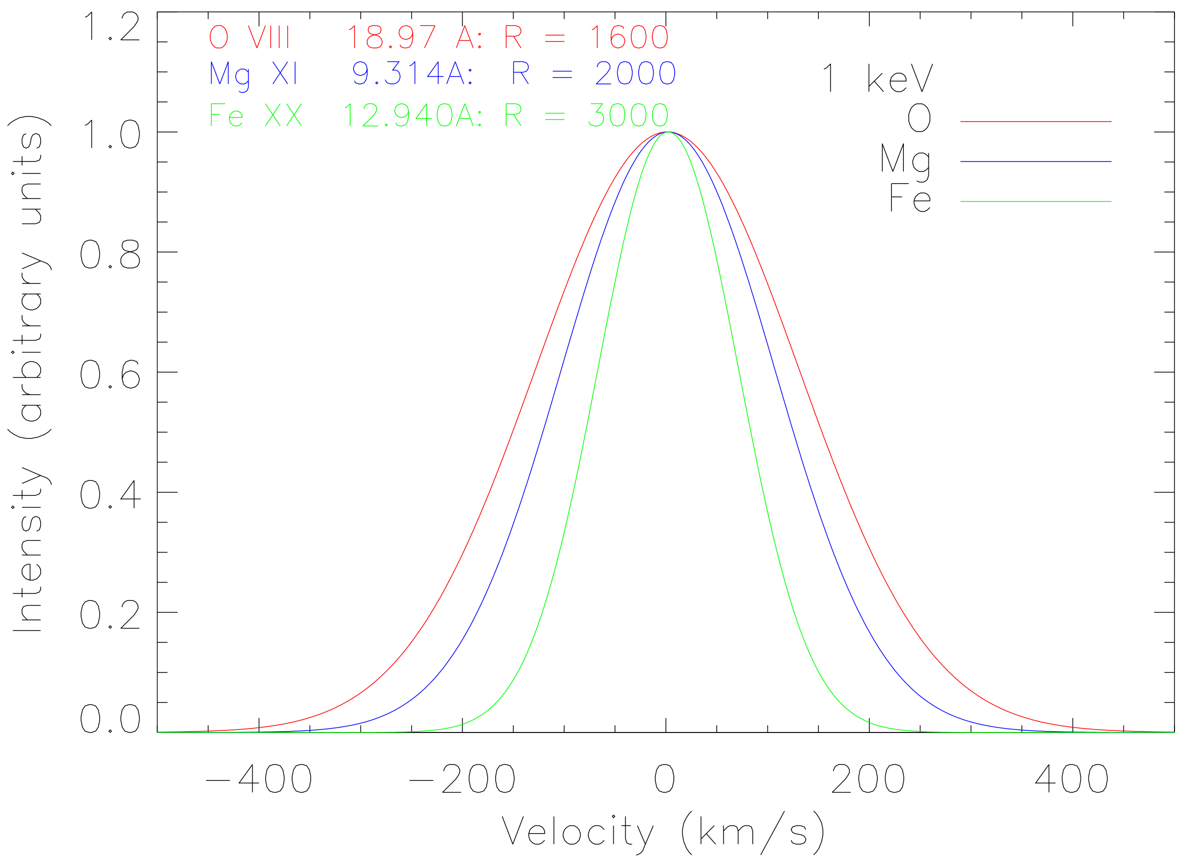
we can use the `mdl2latex` command to get a line list:

```
sherpa> mdl2latex
\begin{tabular}{lllllll}
ModelName & Line Model & Position & Flux & Flux Error & Fit Data & Label \\
 &  & Angstrom & ph/cm$^2$/s & ph/cm$^2$/s &  \\
l1 & delta1d & 15.014 & 0.00308945 & 6.6649e-05 & 3,4,8,9,10,11 &  \\
l2 & delta1d & 15.079 & 0.000269598 & 2.80738e-05 & 3,4,8,9,10,11 &  \\
l3 & delta1d & 15.261 & 0.00125362 & 4.76905e-05 & 3,4,8,9,10,11 &  \\
\end{tabular}
```

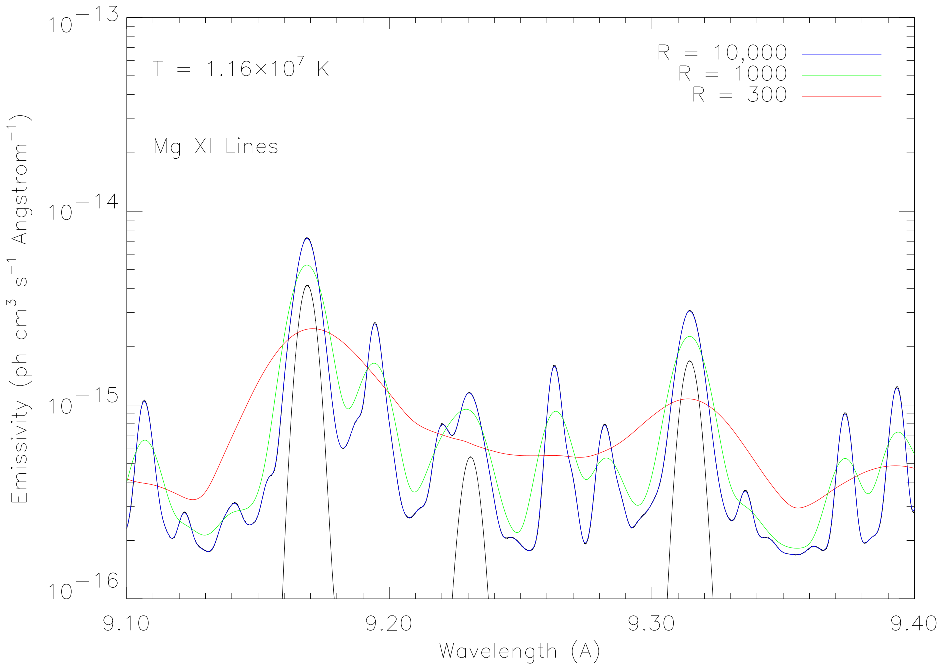
which of course becomes:

Name	Line Model	Position	Flux	Flux Error	Fit Data	Label
		Angstrom	ph/cm^2/s	ph/cm^2/s		
l1	delta1d	15.014	0.00308945	6.6649e-05	3,4,8,9,10,11	
l2	delta1d	15.079	0.000269598	2.80738e-05	3,4,8,9,10,11	
l3	delta1d	15.261	0.00125362	4.76905e-05	3,4,8,9,10,11	

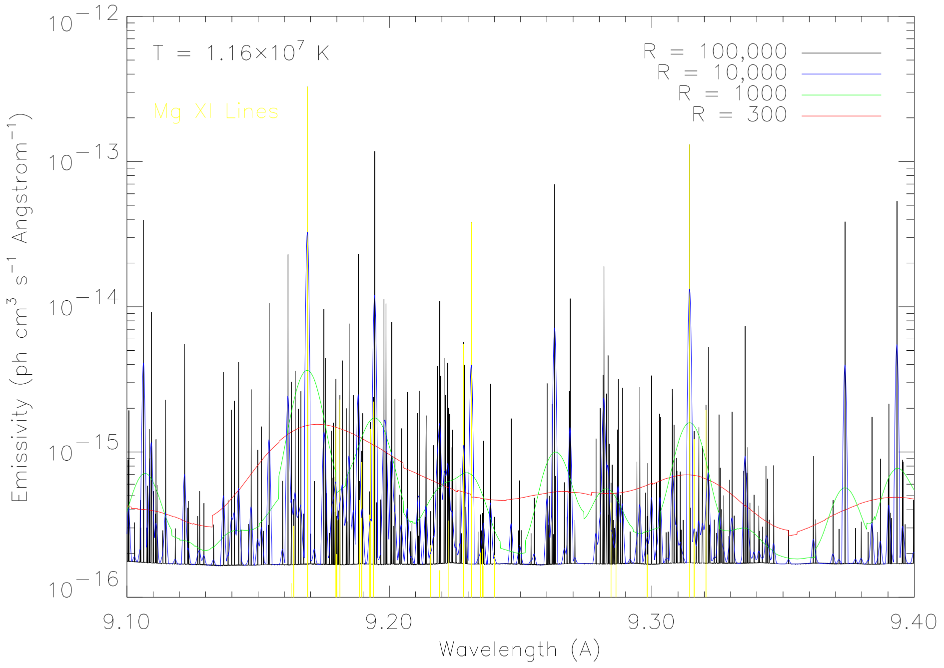
Thermal broadening becomes substantial at relatively low resolution. Some ground-based telescopes have optical spectrographs which can reach resolutions of 1,000,000; for X-ray spectra this would be almost useless, since thermal broadening will be much larger:



Of course, that doesn't mean additional resolution is useless, as shown here:



Without thermal broadening, we see a very different story:



Good news:

- The atomic models for strong lines are in general good to 10-30%, with some important caveats.
- CIAO 2.2 contains a number of new features that will make spectroscopic analysis much easier.
- Adjusting wavelengths dramatically improves fits, and is done for most of the strong Fe L lines and the H, He-like lines.

Warnings:

- More work needs to be done. 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.
- When using line ratios as diagnostics, it is very important to understand what atomic data is being used

And on the observational side, remember how lucky we are:

Pre-Chandra/XMM:

Post-Chandra/XMM: