Atomic Physics, Diagnostics and Uncertainties

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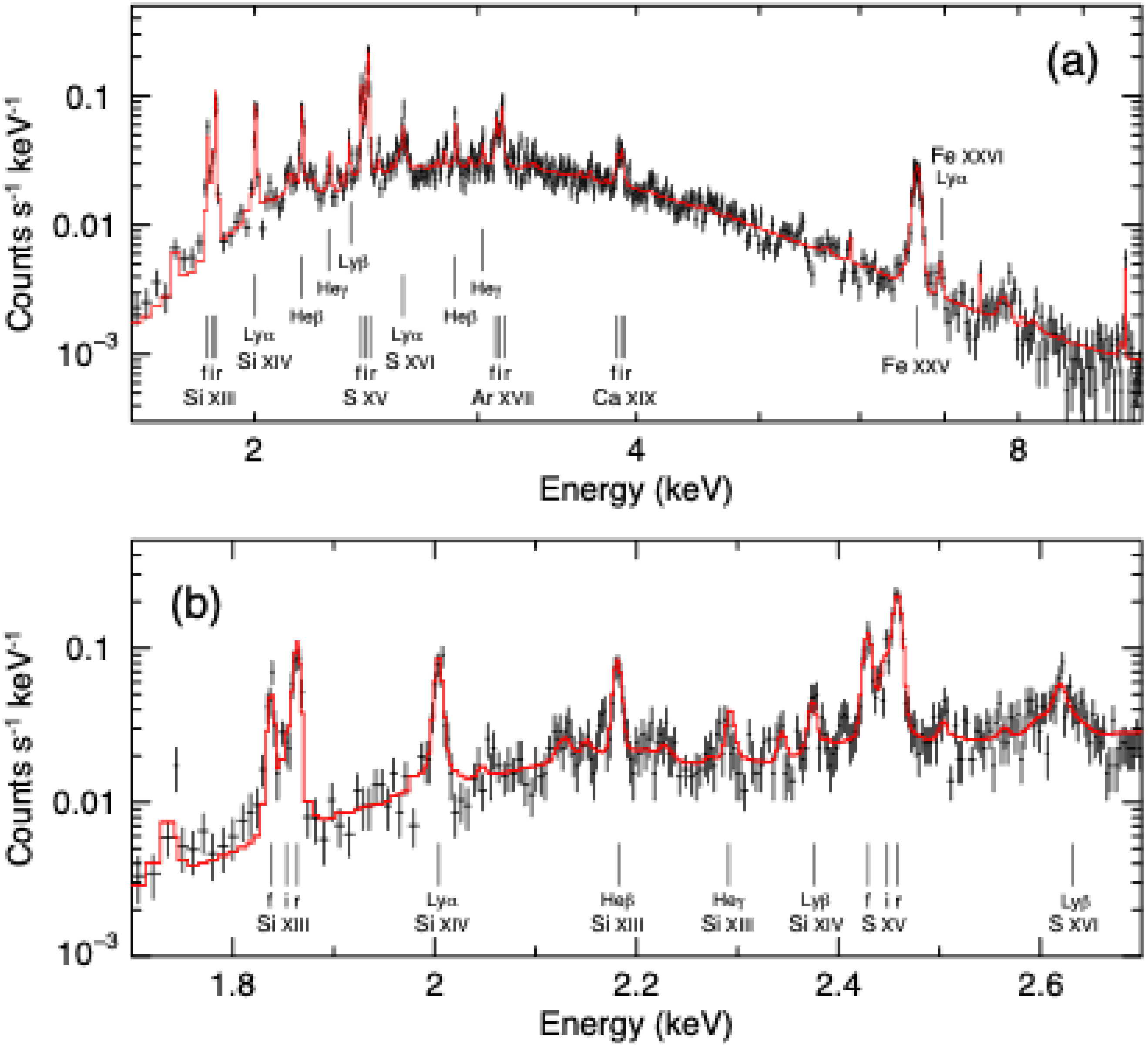
Outline

- Why spectra?
    - Atomic physics is common to all
    - Physical processes in X-ray gas
    - Models are needed which take into account all of them
    - What are the standard physical assumptions,
    - Scope of the problem: how big
    - Atomic data sources
- What are the most widely used codes
- How do we make sure we are getting the right answers: potential pitfalls,
    - Incompleteness
        - Perseus
    - Missing physics
        - X1817
- How do we make sure we are getting the right answers: checking,
    - Code comparisons
    - Experiments
    - Including errors
- Unknown unknowns: energetic particles, non-maxwellian velocity distributions, time variability

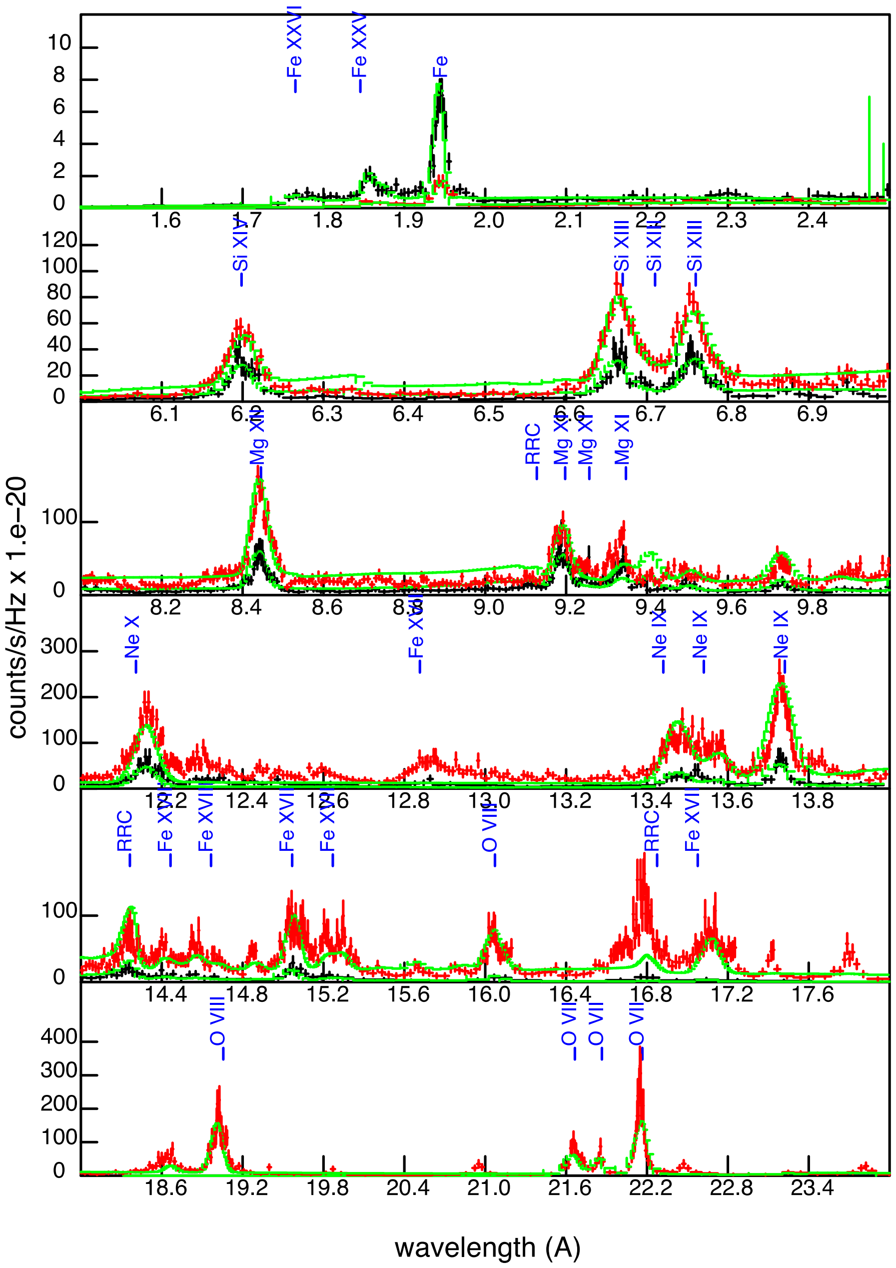
N132D

Supernova remnant with rich array of emission lines



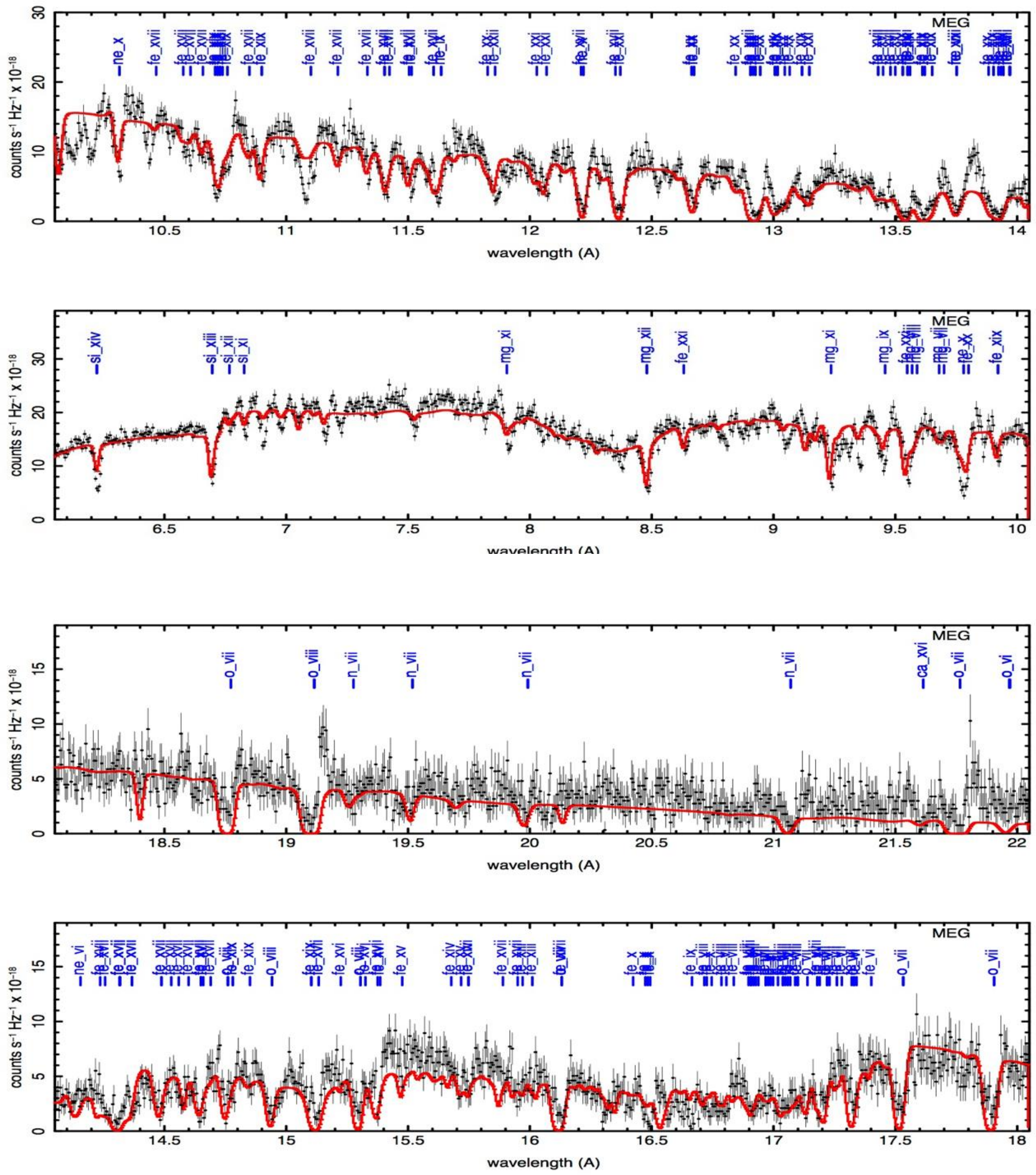
NGC1068

AGN with rich array of emission lines



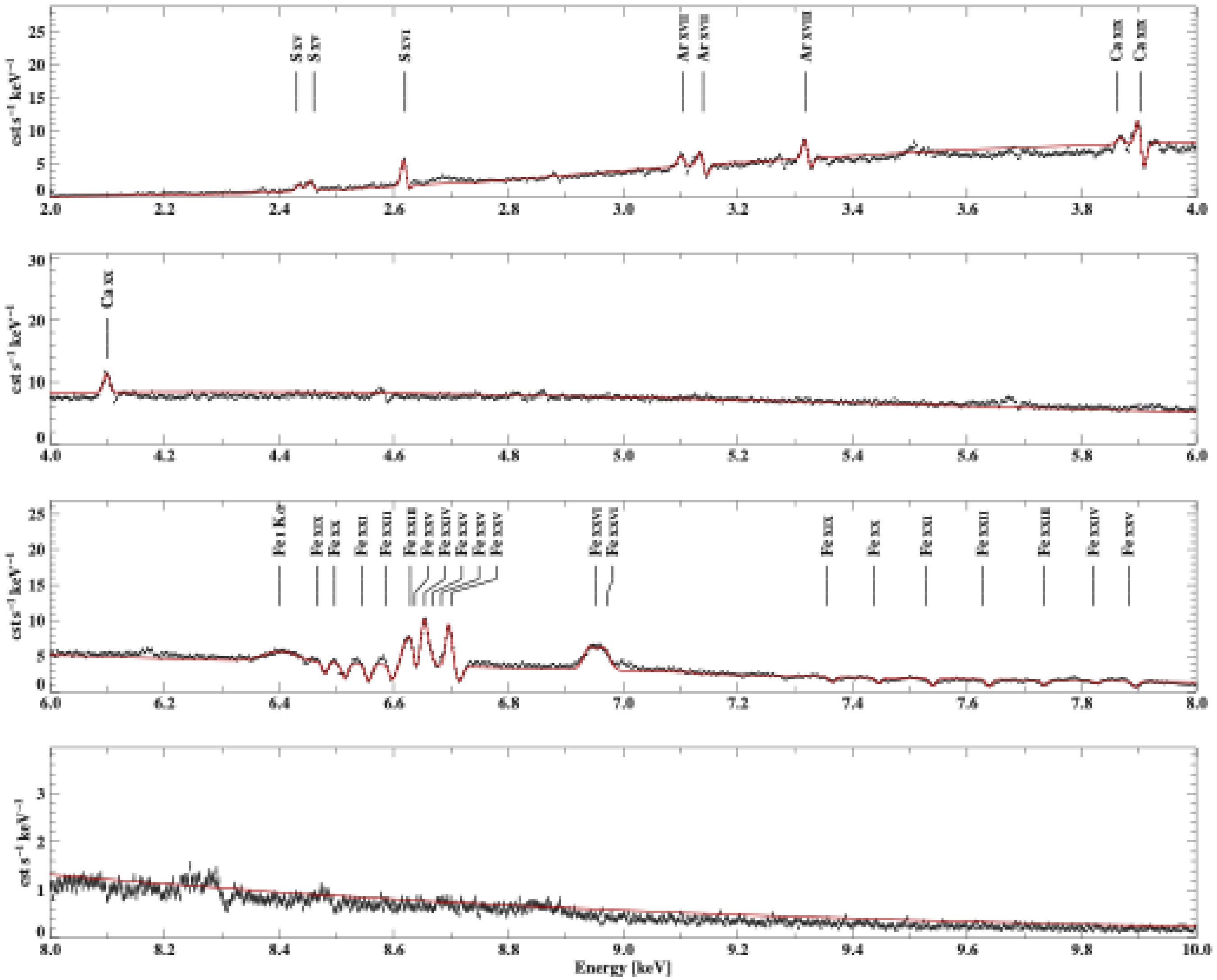
NGC3783

AGN with rich array of absorption lines



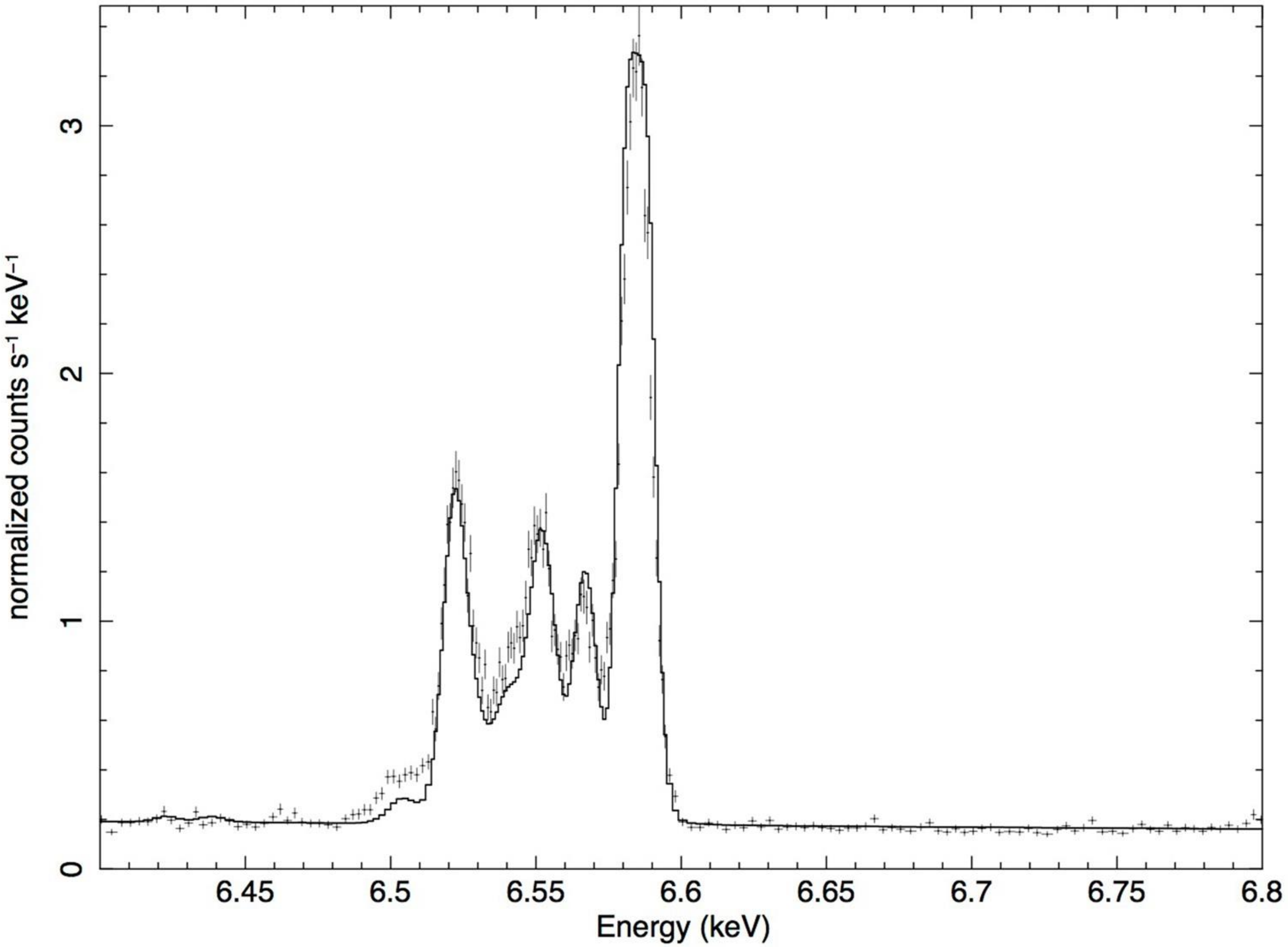
Cyg X-3

Emission and absorption from source with strong continuum from compact source



Perseus Cluster

Iron K line emission (Fe XXV) from hot gas



Atomic Physics Primer:
Hydrogenic energy levels: Bohr atom

$$E_n = -\frac{Z^2}{n^2} \times 1\text{Ry}$$ Energy levels are described by principle quantum number n=0, 1, 2,...

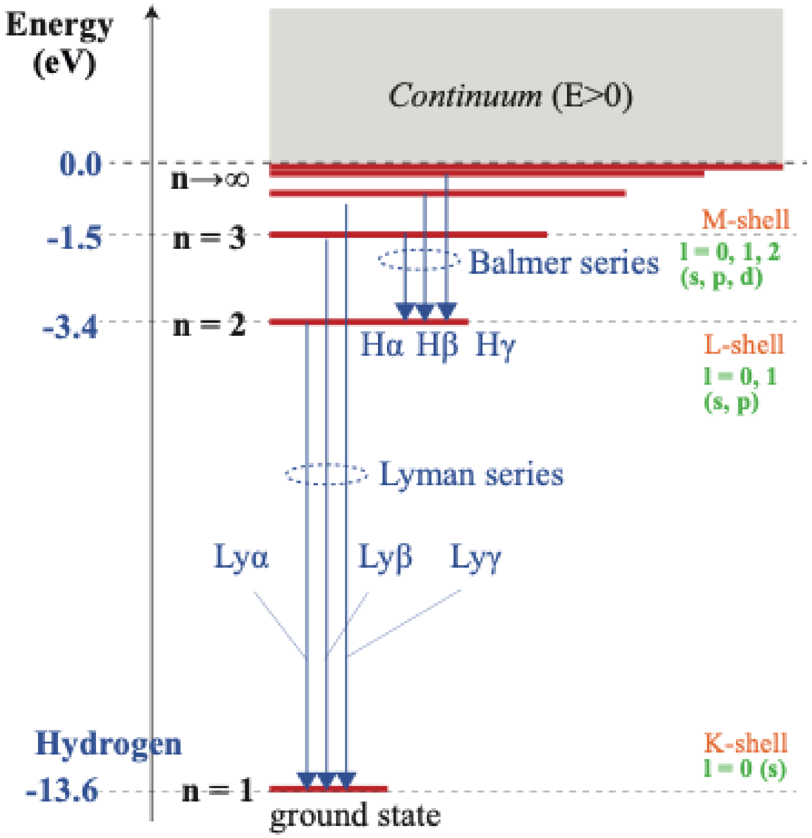


Figure 1: Atomic energy levels of the H-like atom.

Atomic Physics Primer: Multi-electron atoms

As electrons are added, they fill the levels, similar to hydrogenic

Table 2: Electron configuration.

	1s	2s	2p	3s	3p	3d	Configuration
n	1	2		3			
l	0	0	1	0	1	2	
1	1						$1s$
2	2						$1s^2$
3	2	1					$1s^22s$
4	2	2					$1s^22s^2$
5	2	2	1				$1s^22s^22p$
6	2	2	2				$1s^22s^22p^2$
7	2	2	3				$1s^22s^22p^3$
...							
10	2	2	6				$1s^22s^22p^6$
11	2	2	6	1			$1s^22s^22p^63s$
...							
18	2	2	6	2	6		$1s^22s^22p^63s^23p^6$
19	2	2	6	2	6	1	$1s^22s^22p^63s^23p^63d$

Atomic Physics Primer:
Angular momentum and spin

- Also important is the total spin and orbital angular momenta, denoted S and L. These are vector sums of the individual electrons.

$$\vec{L} = \sum_i \vec{l}_i, \quad \vec{S} = \sum_i \vec{s}_i, \quad \vec{J} = \vec{L} + \vec{S}$$

(configuration) $^{2S+1}L_J$

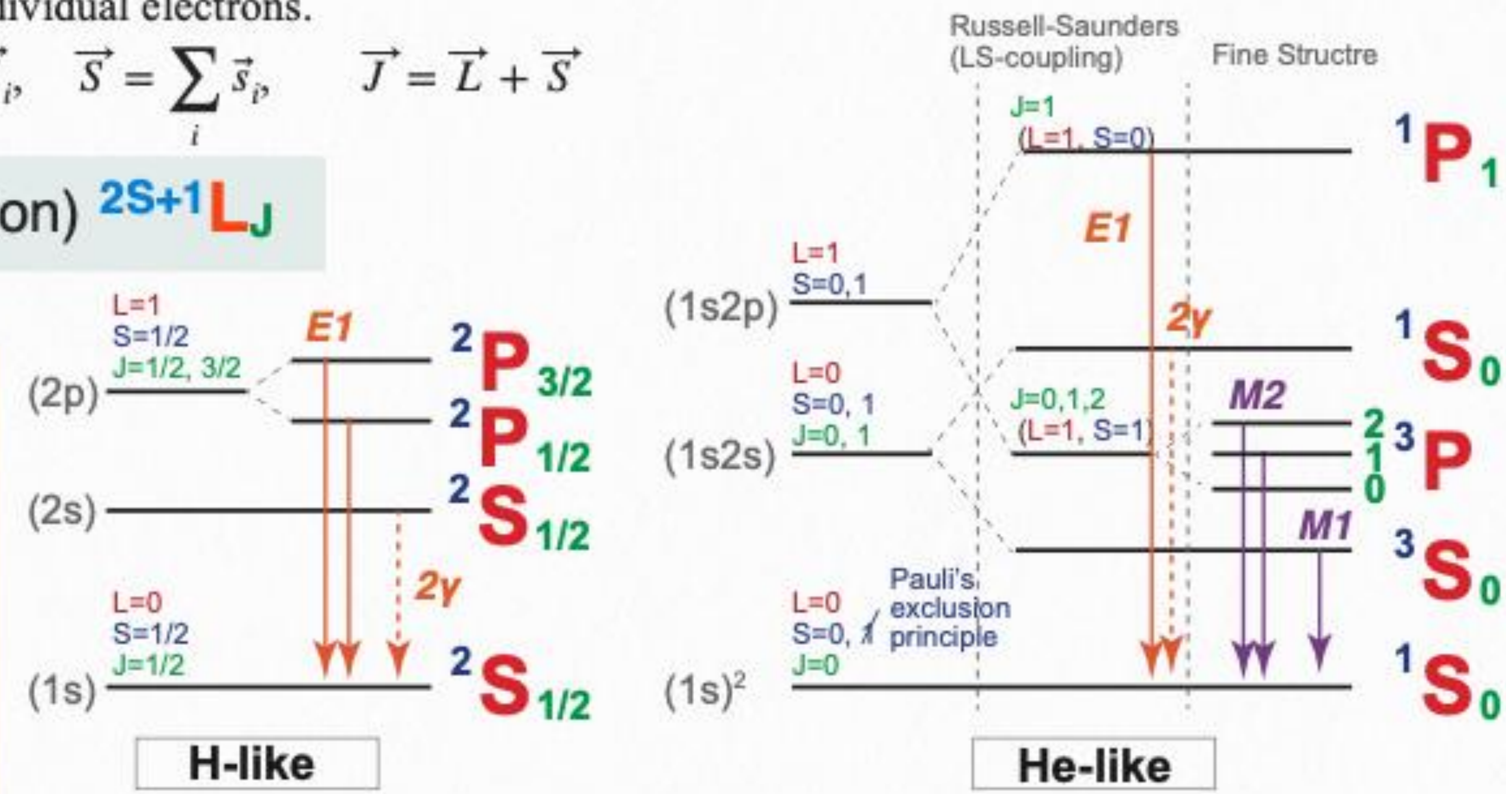


Figure 2: Schematic diagram of energy levels of H-like and He-like ions.

Selection rules (initial/final states of permitted transition)

$\Delta l = \pm 1$, $\Delta m = 0, \pm 1$, $\Delta S = 0$, $\Delta L = \pm 1$, $\Delta J = 0, \pm 1$ (except J=0 to J=0)

What happens in X-ray gas?

1) Photoionization: $\sigma \sim \pi a_0^2 Z^{-2}$

   Need photon energy ~1RyZ^2 ~ 0.8 keV eg. for oxygen

2) Inelastic Electron-ion collisions: $\sigma \sim \pi a_0^2 Z^{-2}$

   Need electron energy kT ~1RyZ^2~10^7K eg. for oxygen

3) Recombination: comparable cross section, no threshold

4) charge transfer: $\sigma \sim \pi a_0^2$ → large for low ionization projectiles

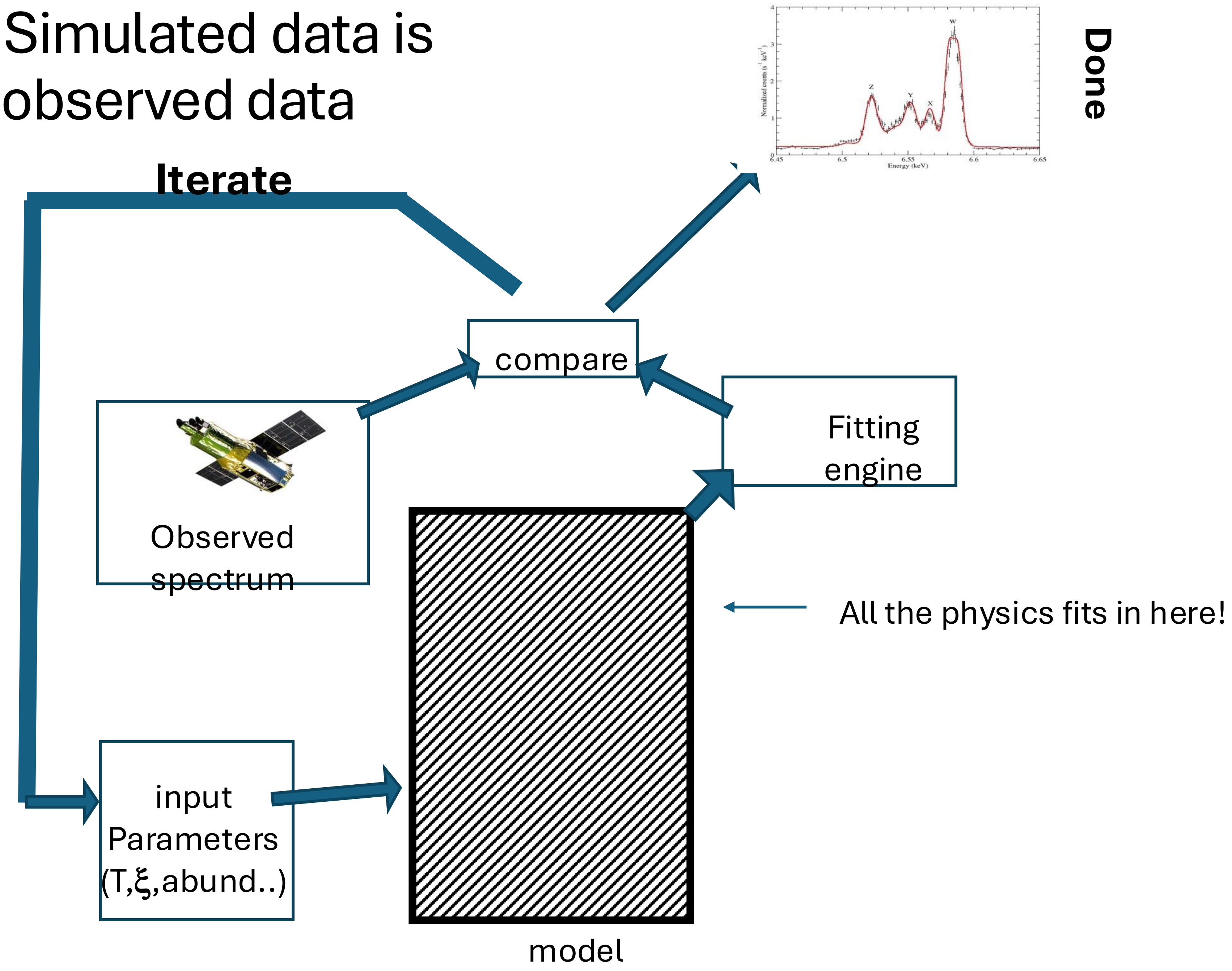
→ which ones win depends on conditions: T, radiation field, neutrals

Modeling X-ray plasmas involves consideration of all of these processes

Process	inverse	Heating/cooling	Emission/absorption
Photoionization	Radiative Recombination	y	y
Photoexcitation	Radiative decay		y
Autoionization	Dielectronic recombination	y	
Electron impact excitation	Electron impact deexcitation	y	
Electron impact ionization	3 body recombination	y	
Charge transfer (ionization)	Charge transfer (recombination)	y	
Bremsstrahlung	Free-free absorption	y	y
Compton scattering	Inverse Compton	y	y

- Physically accurate models need to calculate the effects of *all* these processes.
- All are coupled thru temperature

Typical model procedure involves iterative fitting. Simulated data is compared with observed data



Most models employ a standard set of physical assumptions

- Maxwellian electron velocities, single temperature
- At most marginally optically thick
- Time steady (or not)
- Simple geometry: slab or sphere
- ~Cosmic element abundances
- Weak radiation field → neglect stimulated processes

Even with these simplifications, modeling spectra is challenging.

- ~30 elements
- ~465 ions
- 10-100 levels per ion → ~10^5 levels
- 100-1000 lines per ion → ~10^6 lines
- Statistical equilibrium: rate in=rate out
  - → A large coupled linear system ~10^5 equations

$$\frac{dn_i}{dt} = \Sigma_j \left(n_j R_{ji}(T, F, n..) - n_i R_{ij}(T, F, n...)\right)$$

- Plus radiative equilibrium in some cases

$$\frac{d}{dt}\left(\frac{3}{2}nkT\right) = H(T, F, n..) - C(T, F, n..)$$

- Plus radiative transfer
- → atomic database contains ~(465)x(100)x(100) real numbers~8x10^8 ~3Gbytes ascii
- Where to get all this data? How to check it? Is it accurate enough?

Modeling codes

- Photoionization equilibrium (xstar/warmabs, cloudy, pion)
- Coronal equilibrium (apec, spex, chianti)
- Non-equilibrium ionization (apec, spex)
- Charge exchange (apec, spex)
- Time dependent photoionization (pion, xstar)

Some codes are directly callable from xspec or spex (` analytic' models)
Others use tables: mtables or atables

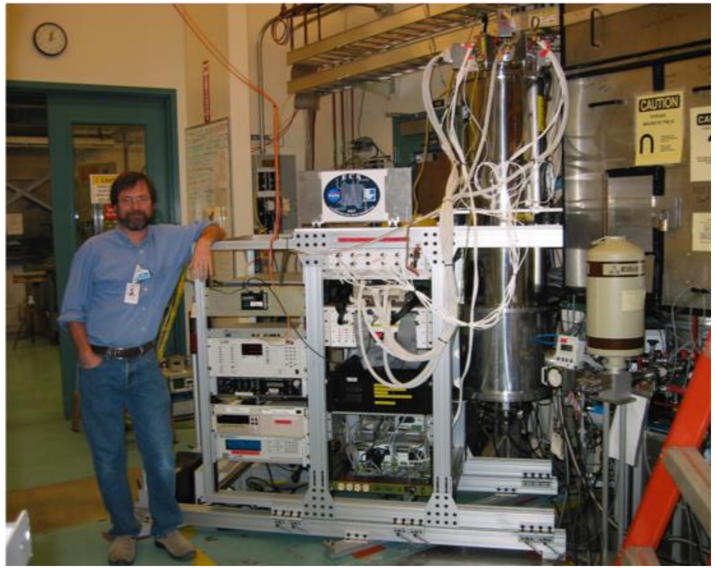
Where do rates and other quantities needed for modeling come from?

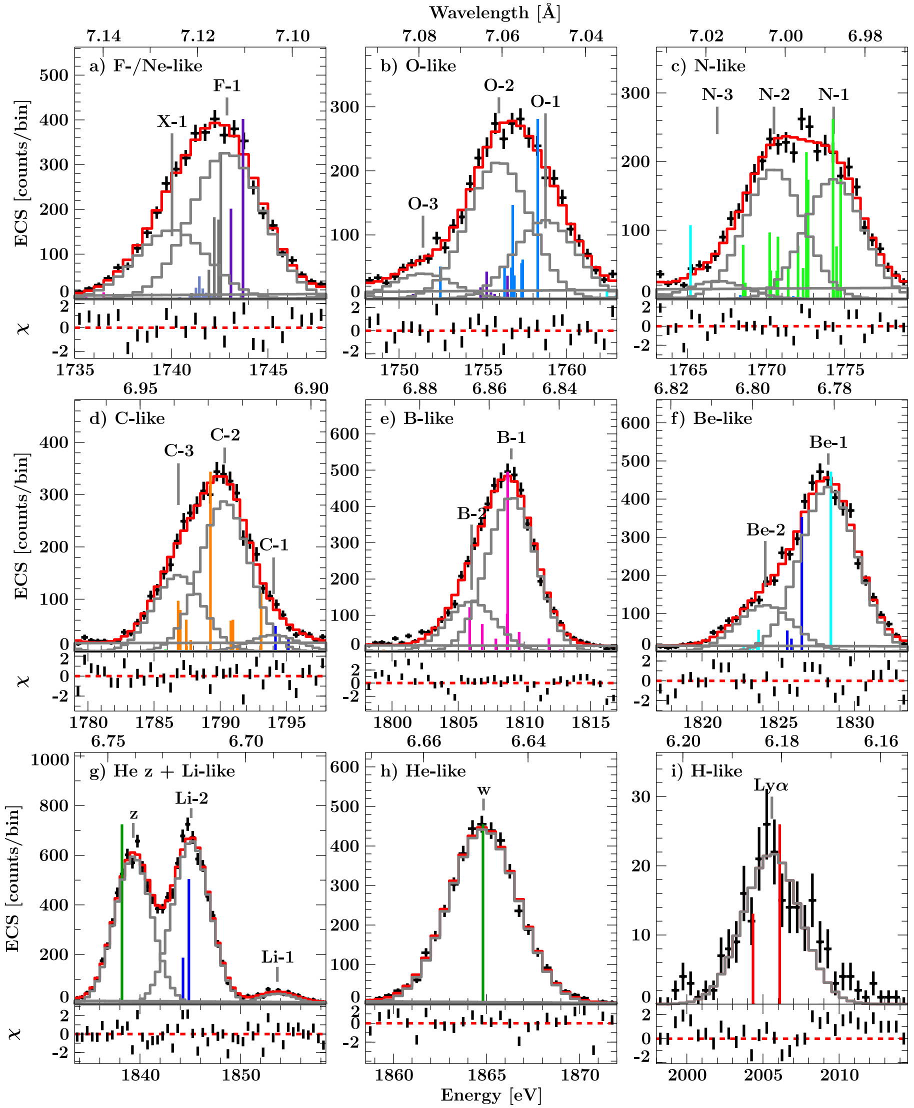
- Atomic calculations are the only practical source for most quantities
- Approximations:
  - Configuration interaction
  - Hartree-fock (MCHF)
  - Dirac or dirac-fock: (MCDF)
  - Breit-pauli
  - Multi-body perturbation theory (MBPT)

$$H = \sum_{i=1}^{N}\left[-\nabla_i^2 - \frac{2Z}{r_i}\right] + \sum_{j\neq i}\frac{2}{r_{ij}}.$$

- Scattering packages:
  - Distorted wave
  - R-matrix
- Structure packages:
  - Fac/hullac
  - autostructure

Experimental measurements are potentially the most accurate





Hell et al. 2016

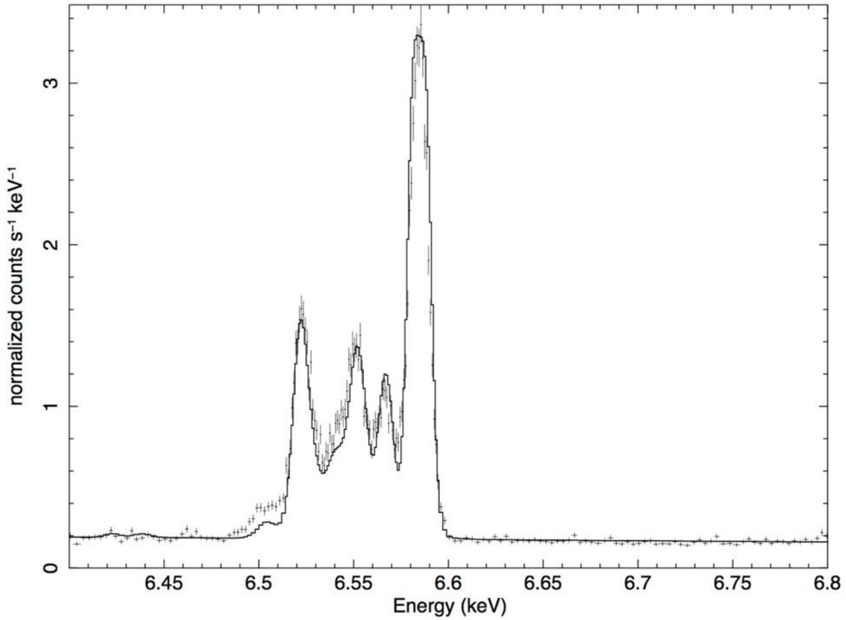
Line energies can be used to benchmark calculations

Atomic data accuracy: rules of thumb

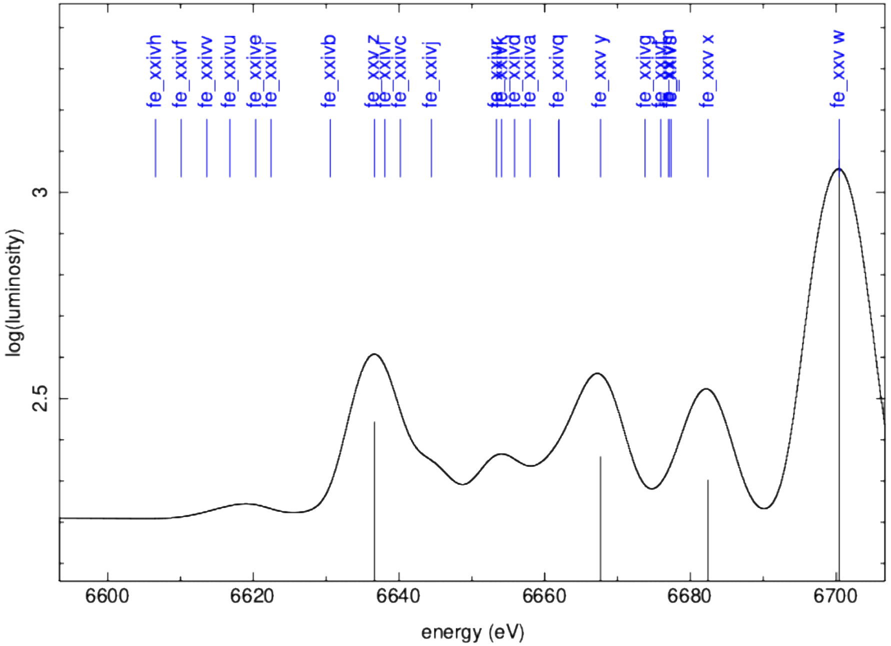
- Calculations:
  - Rates/cross sections: 10-20%
  - Energy levels: ~1%
  - mbpt claims ~0.1%
- Measurements
  - Energy levels: 0.1% or better
  - Rates/Cross sections: ~1% (?)

Atomic data Completeness: Hitomi spectrum of the Perseus cluster

- Model fit to Hitomi spectrum of Perseus
- Shows expected He-like lines

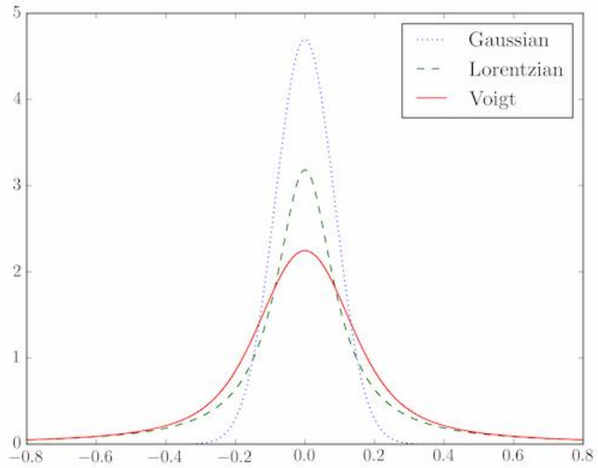


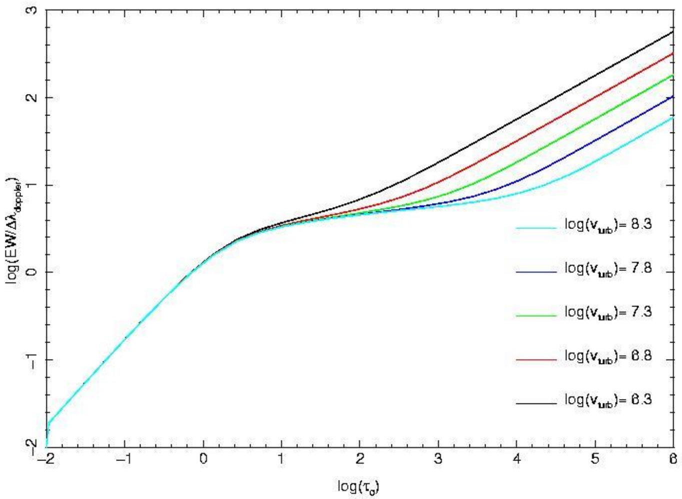
- Log plot shows weaker lines from Li-like Fe contributing to fit



Atomic data Completeness: the importance of damping on X-ray lines

- Optical and uv lines generally involve excitation from the valence shell
  - → decay is the opposite of excitation,
  - upper level lifetime scales ~z^{-4} or E^{-2}
- X-ray lines often involve inner shells
  - Decay can occur by autoionization
  - Decay rate scales ~z^{0}
  - → at Z<30 autoionization can be dominant
- If so, line shape has different character
  - This is called *Auger damping* or *Non-radiative damping*.
  - Correct line profile is Voigt profile: Gaussian core, Lorentzian wings.
  - The damping parameter can be much larger than for optical/UV lines





Atomic data completeness: lifetimes of inner shell vacancy levels

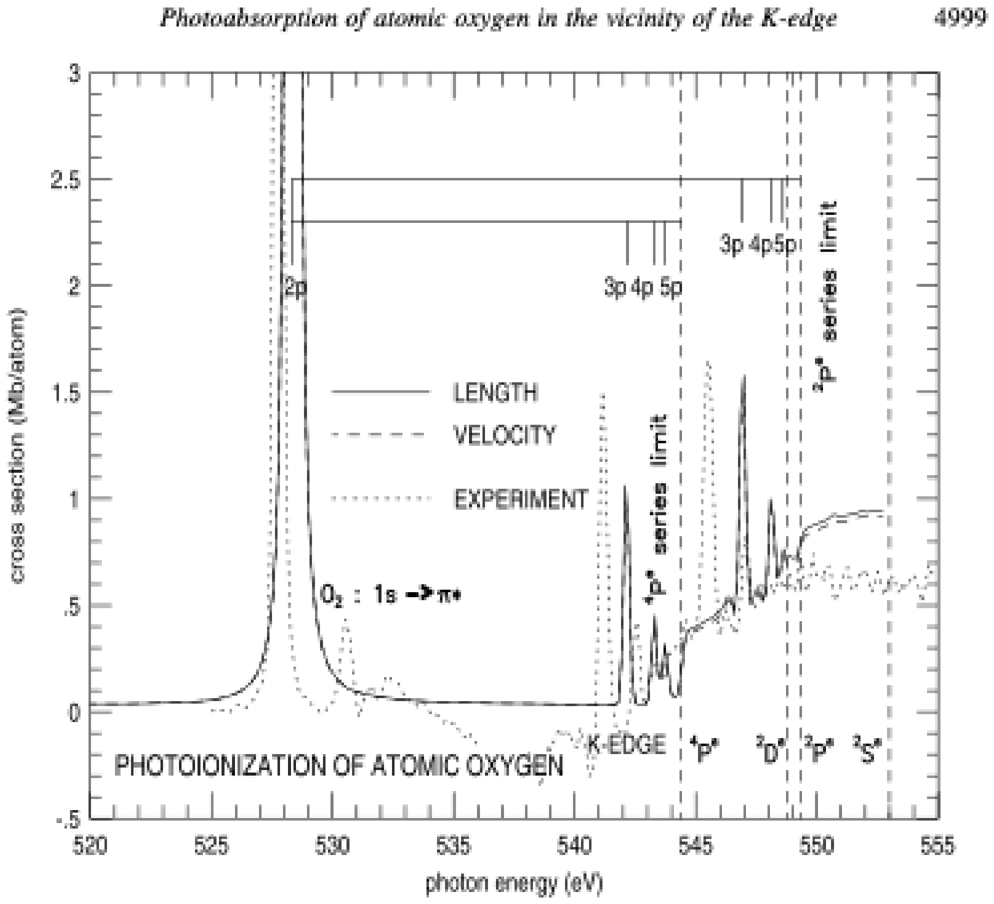
- Lifetime of excited levels depend on sum over many possible decay channels
- These include radiative and non-radiative channels
- Non-radiative channels
  - Have large rates for many inner shell transitions
  - Do not obey dipole selection rules
  - Are easy to ignore when calculating structure
- Including these channels is crucial to getting accurate lifetimes and fluorescence yields.

Z	N	Level	HFR1 (s^{-1})	AS1 (s^{-1})	HULLAC[a] (s^{-1})
14......................	5	$1s2s^22p^2\ ^2P_{1/2}$	1.63+14	1.67+14	7.58+13
	6	$1s2s^22p^3\ ^3S^o_1$	2.05+14	2.23+14	1.16+14

(Palmeri et al. 2008)

Atomic data completeness:
The photoionization cross section of O I near the K edge

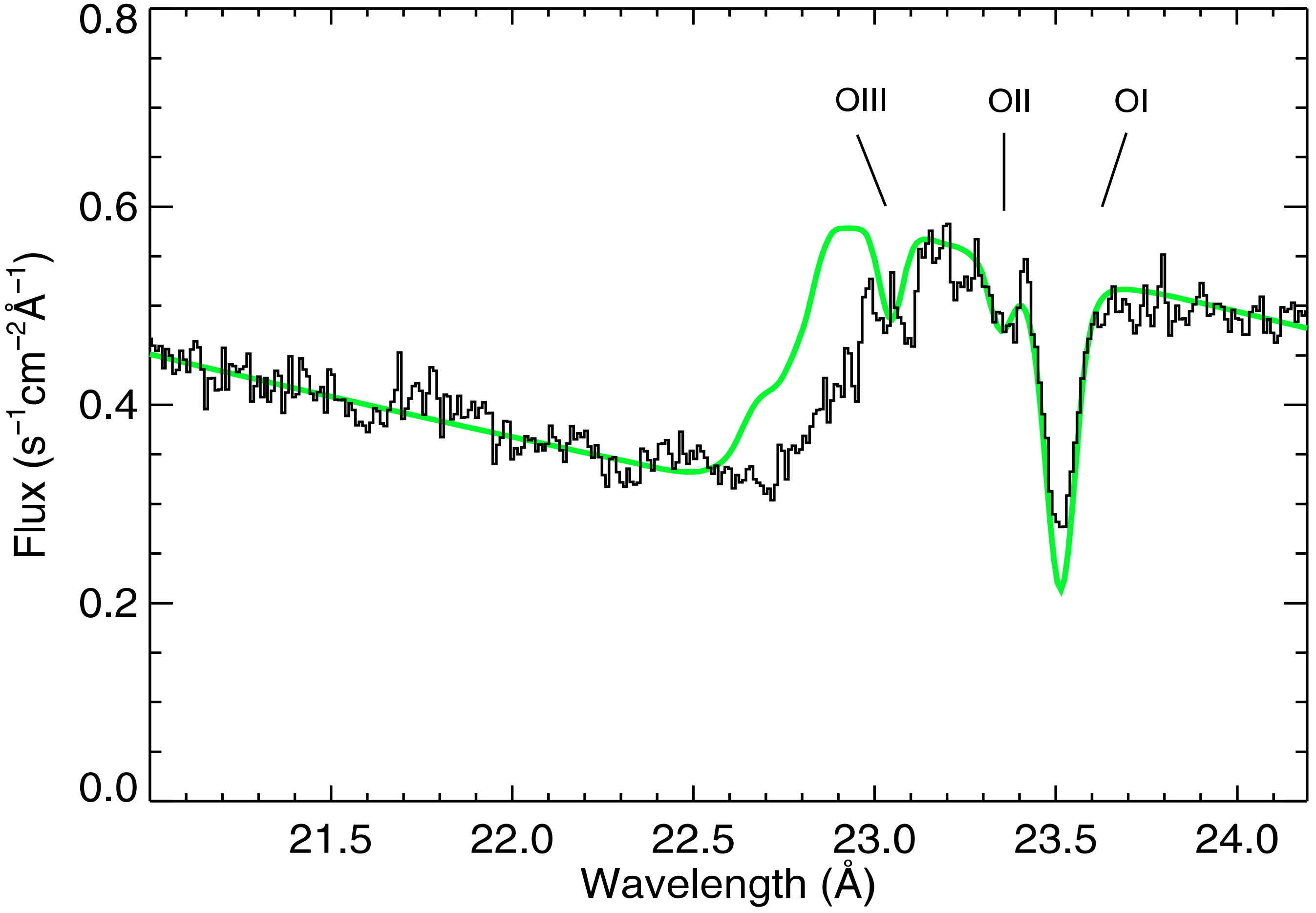
- Early calculations showed resonances near K edge
- $K\alpha >> K\beta$



(Mclaughlin and Kirby 1998)

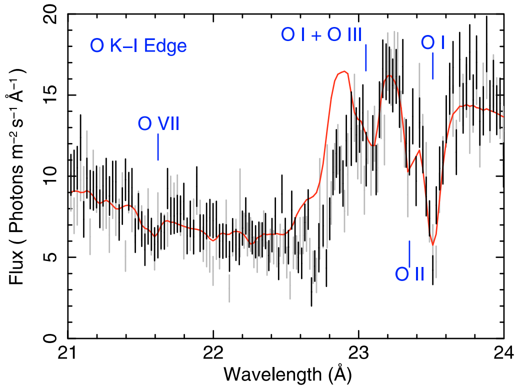
Atomic data completeness: With Chandra this edge was observed

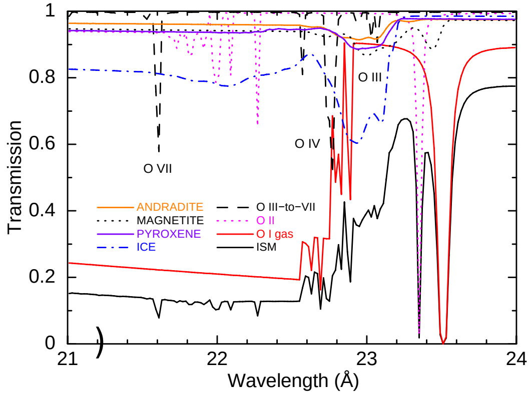
- Chandra HETG Spectrum of Sco X-1
- Shows apparent excess absorption below the K edge

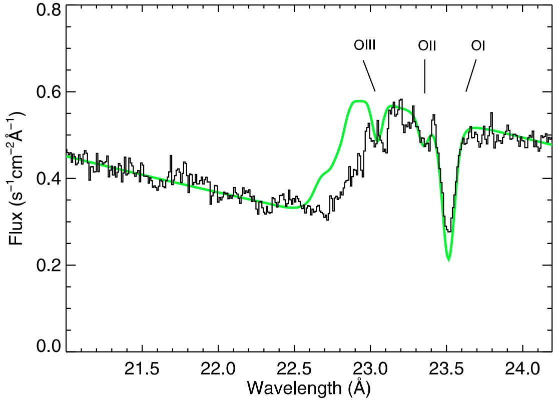


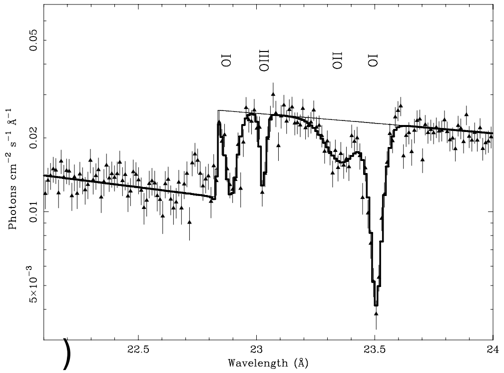
deVries etal (2009)

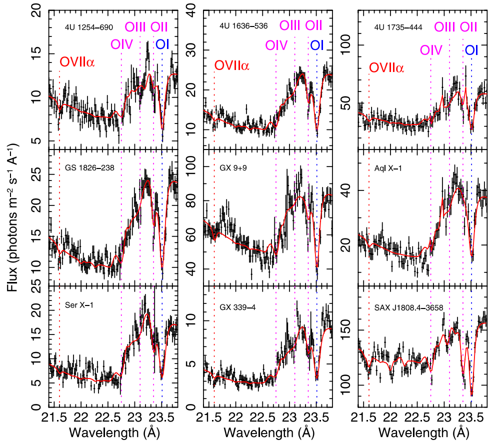
Atomic data completeness:
Similar results were found for other X-ray binary ism spectra

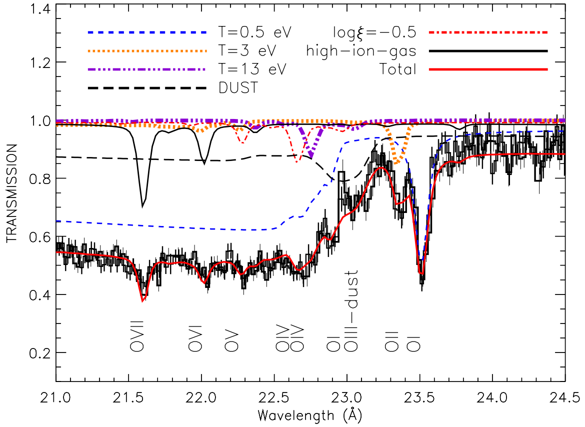












→ Extra absorption appears below the edge

Atomic data completeness:
One hypothesis for the below-edge absorption is molecules

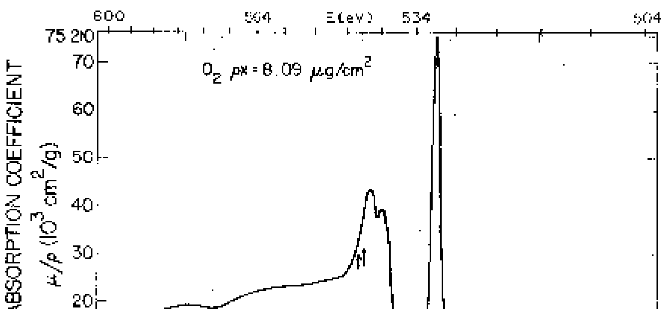
CO: edge near 542eV=22.9A

1058 BARRUS, BLAKE, BUREK,

probable that the weak shake-up transitions are overwhelmed in this range by a potential barrier peak, which in N_2 has been shown quantitatively to reach such large relative intensity by Dehmer and Dill.[16] On the other hand, the appearance of a very

AMBERS, AND PREGENZER 20

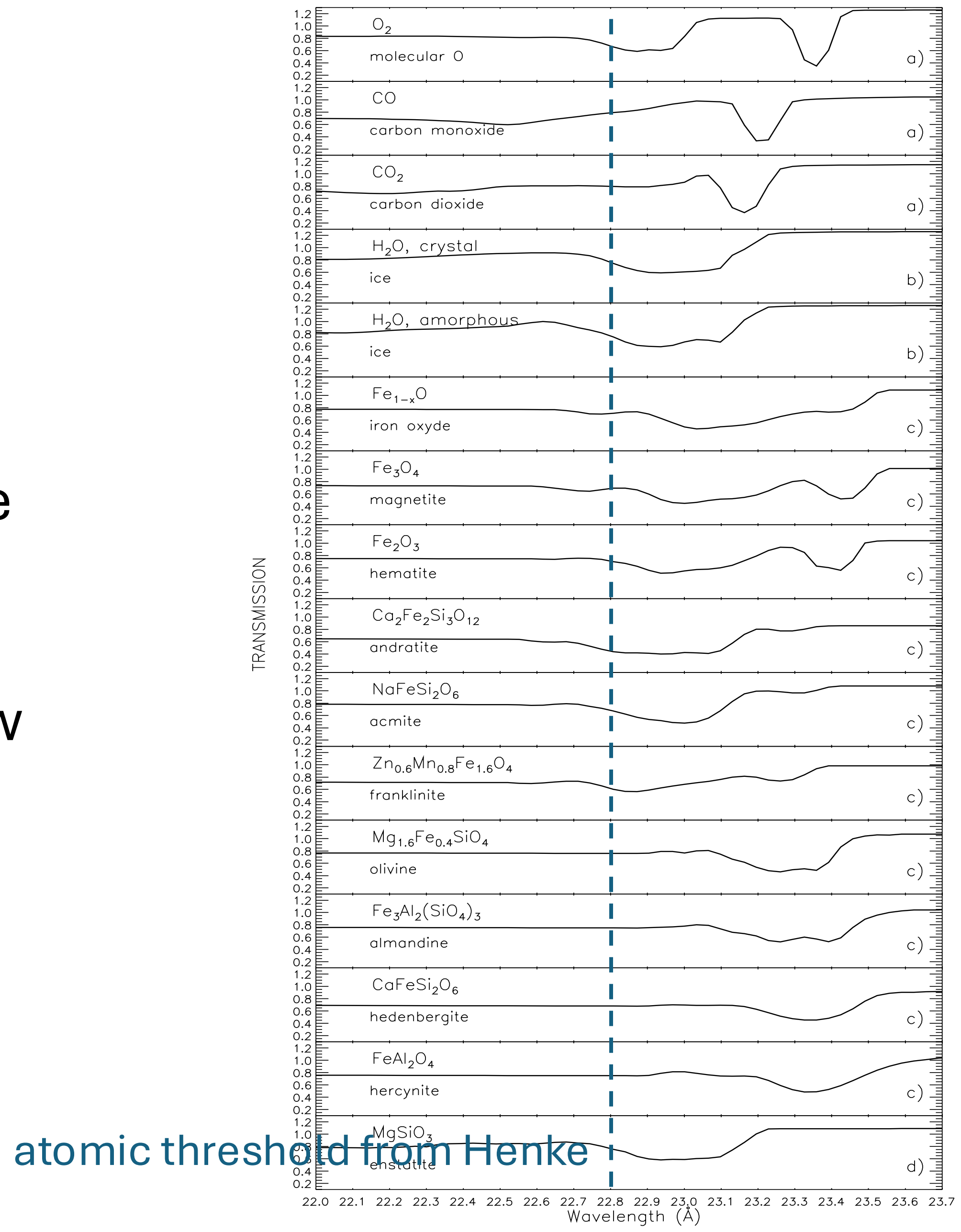
O_2: edge near 537 eV=23.1A



(Barrus et al. 1979)

Atomic data completeness: Lab spectra of some oxygen compounds also show absorption

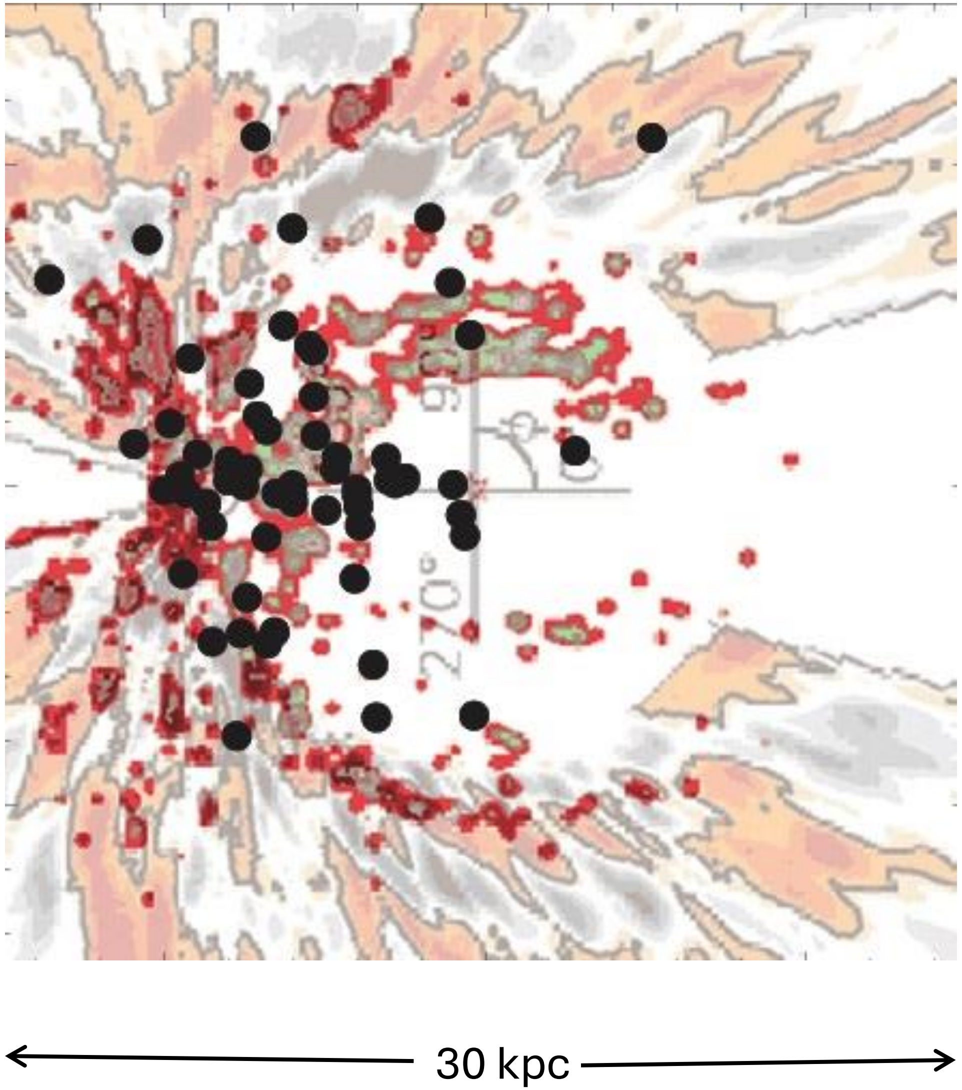
- potential diagnostics of the molecular/solid content of the ISM?
- Essentially all spectra show molecules with column comparable to atomic



(Costantini et al. 2012)

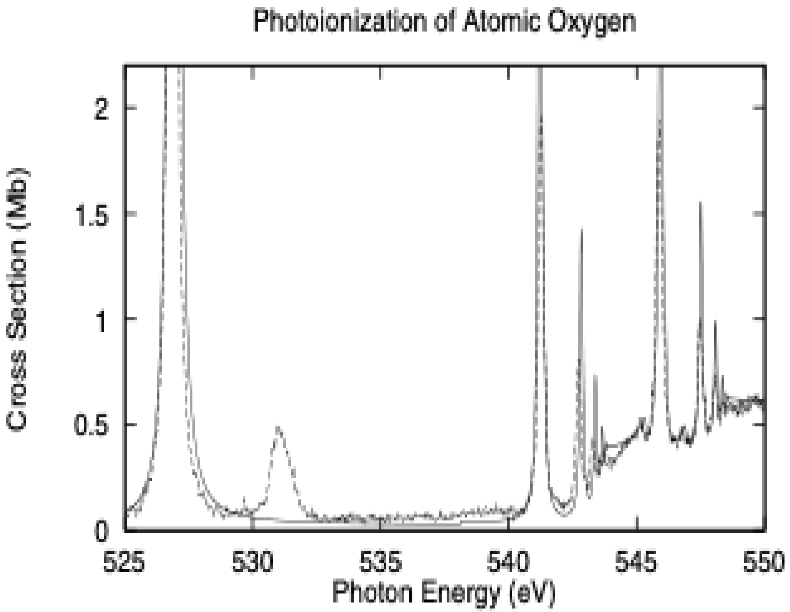
Atomic data completeness: Does it make sense that all lines of sight have molecules?

- X-ray binary sightlines probe significant distances in the galactic plane
- Location of X-ray binary sample overlaid on HII region map (Levine et al. 2006) does not show perfect coincidence
- Expect ~10% filling factor for truly cold molecular material
- So what is going on?



Atomic data completeness: more recent calculations of the photoionization cross section of O I near the K edge

- Resonances near K edge
- $K\alpha$ and $K\beta$ more nearly comparable



(Gorczyca and Mclaughlin 2003)

Atomic data completeness:
The photoionization cross section of O I near the K edge

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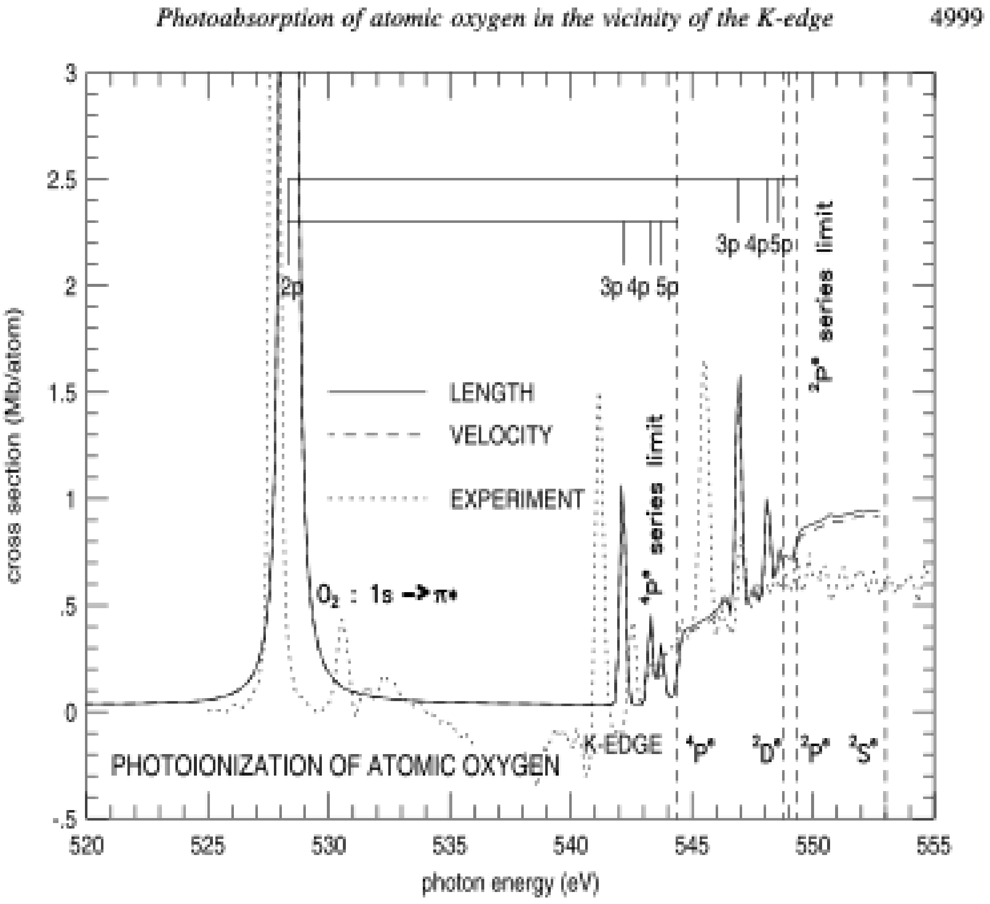
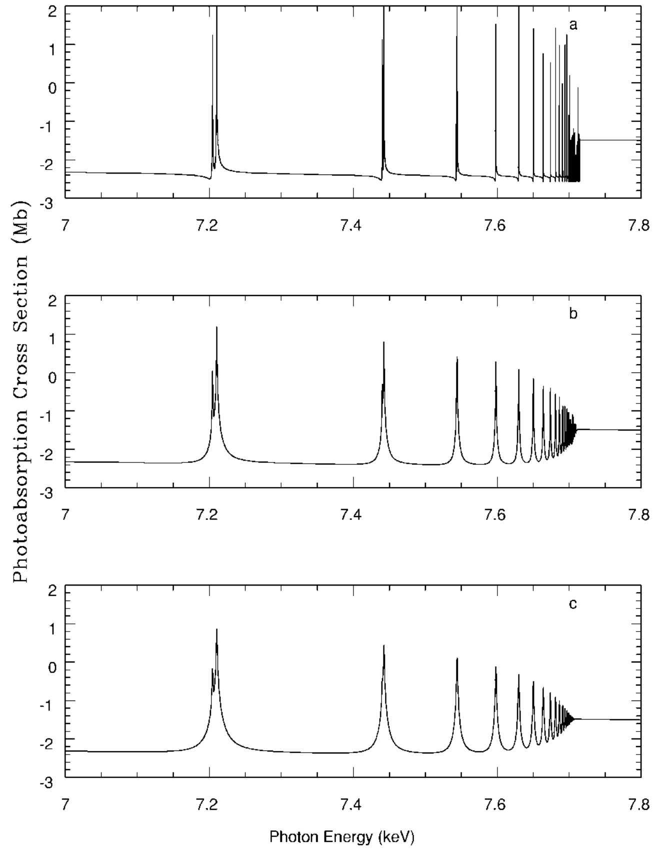


(Mclaughlin and Kirby 1998)

Atomic data completeness: Here is why Kα~ Kβ :

- K shell resonances (1s-np) close to threshold can decay by an alternate channel.
- Auger decay in which the high n electron does not participate is rapid and independent of n
- This broadens the resonances and causes them to blend and smear the edge
- In such 'spectator Auger' decay the Rydberg electron does not participate in the decay
- This is important for ions with more than 3 electrons



(Palmeri et al. 2003)

$$h\nu + 1s^2 2s^2 2p^4 \rightarrow 1s2s^2 2p^4 np,$$

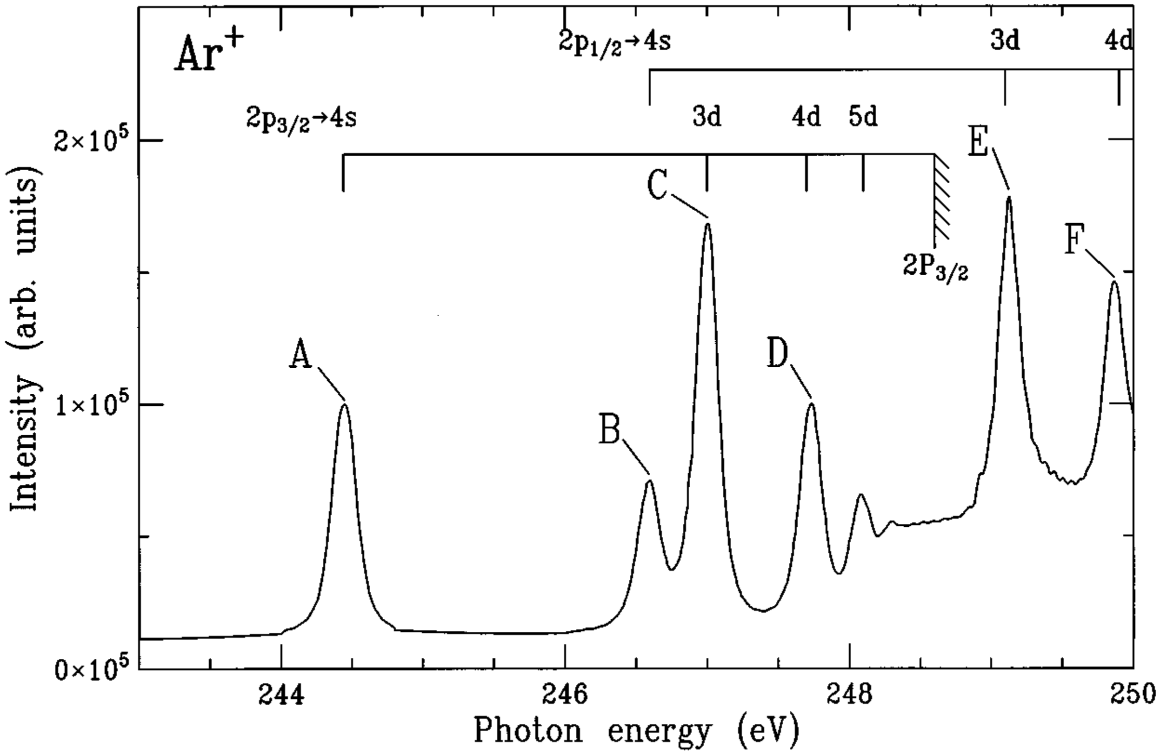
participator

$$1s2s^2 2p^4 np \rightarrow 1s^2 2s^2 2p^3 + e^-$$
$$\rightarrow 1s^2 2s2p^4 + e^-,$$

spectator

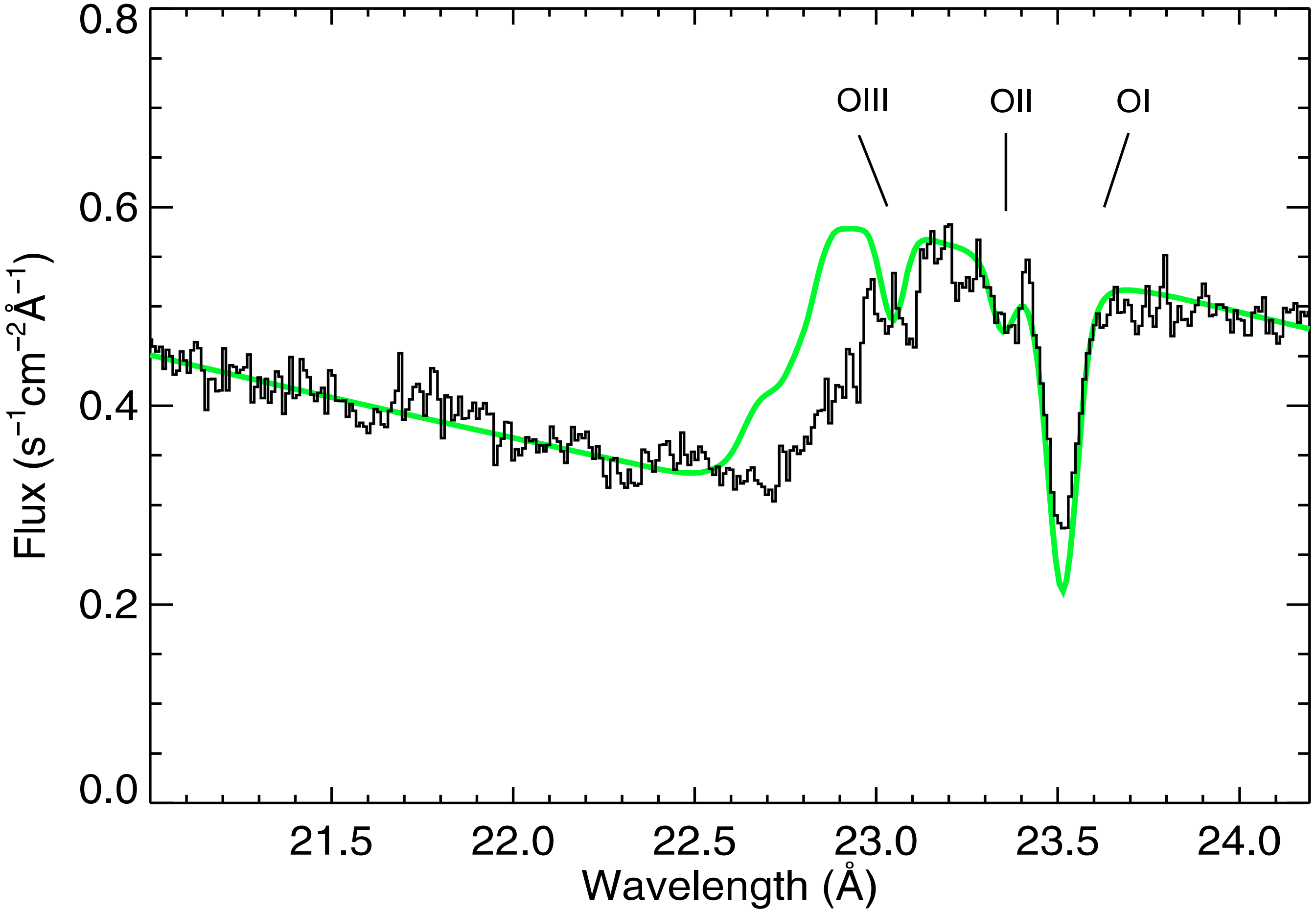
$$1s2s^2 2p^4 np \rightarrow 1s^2 2s^2 2p^2 np + e^-$$
$$\rightarrow 1s^2 2s2p^3 np + e^-$$
$$\rightarrow 1s^2 2p^4 np + e^-,$$

Atomic data completeness: Experimental Demonstration of Auger damping in Ar+



(Farhat et al., 1997)

Atomic data completeness:
Fit to Chandra observation of O I edge



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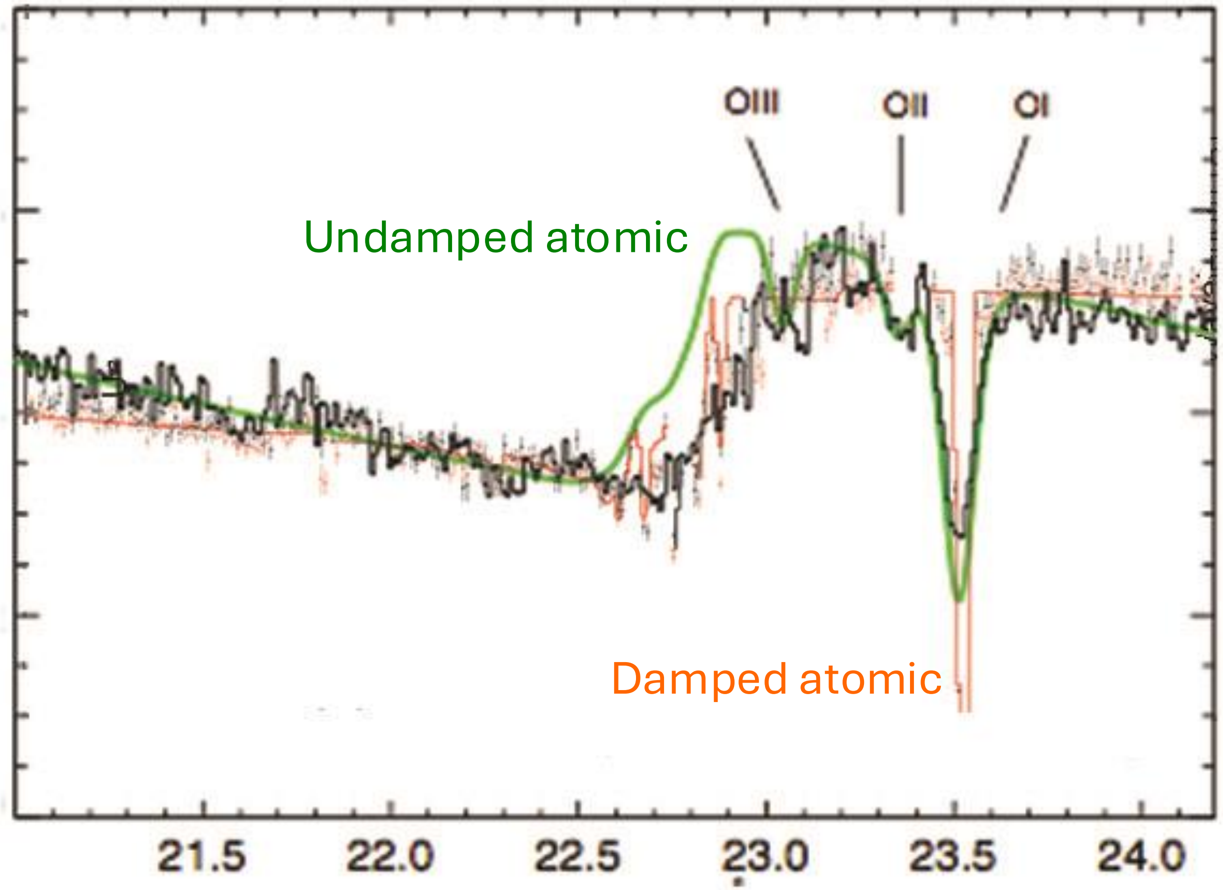
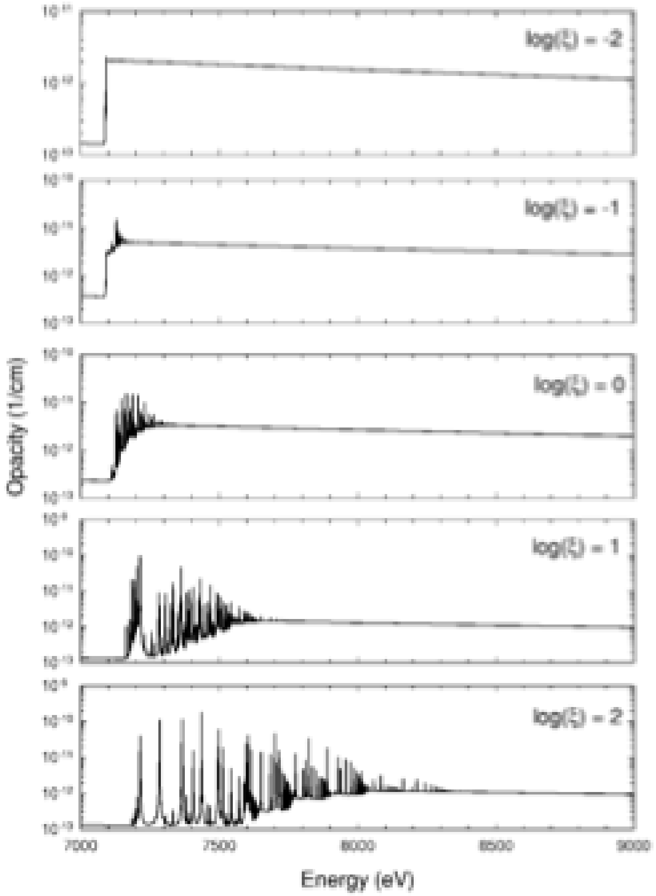


Atomic data completeness:
The effect of Auger damping on the iron K edge

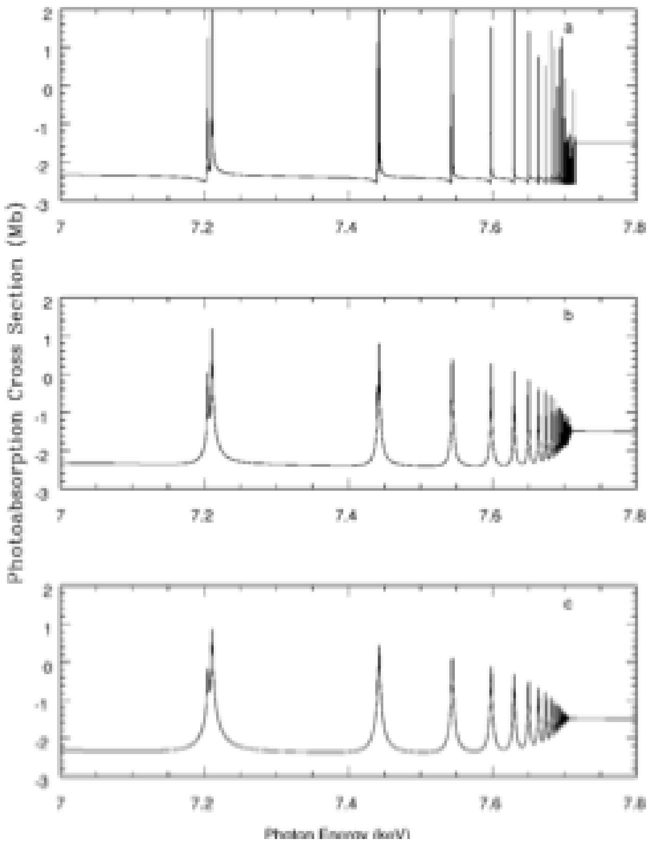


Iron opacity vs. ξ

No damping

Radiative only

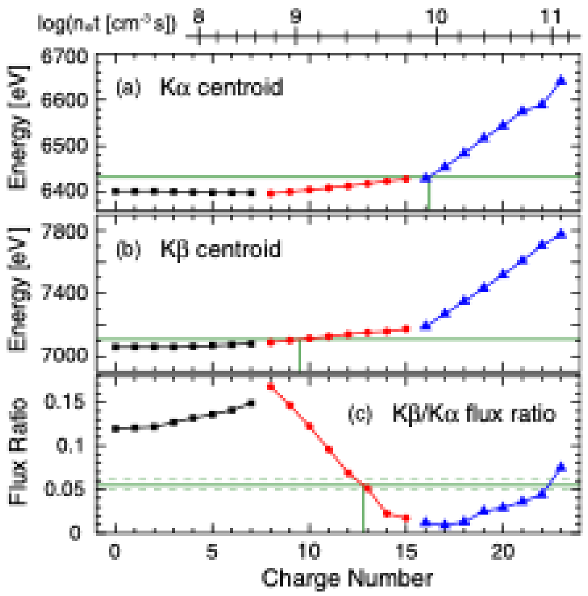
Radiative + Auger



Fe XVII

Atomic data accuracy: Fe K line energies

- For neutral Fe, experimental measurements are accurate to $\Delta\varepsilon/\varepsilon$ ~1.e-4
- For ions near neutral, calculations are all that is available
  - Likely accuracy is $\Delta\varepsilon/\varepsilon$~1e-2.
  - Corresponds to 300 km/s
  - But they agree with experiment for neutral to within 1.e-4



Yamaguchi et al. 2012

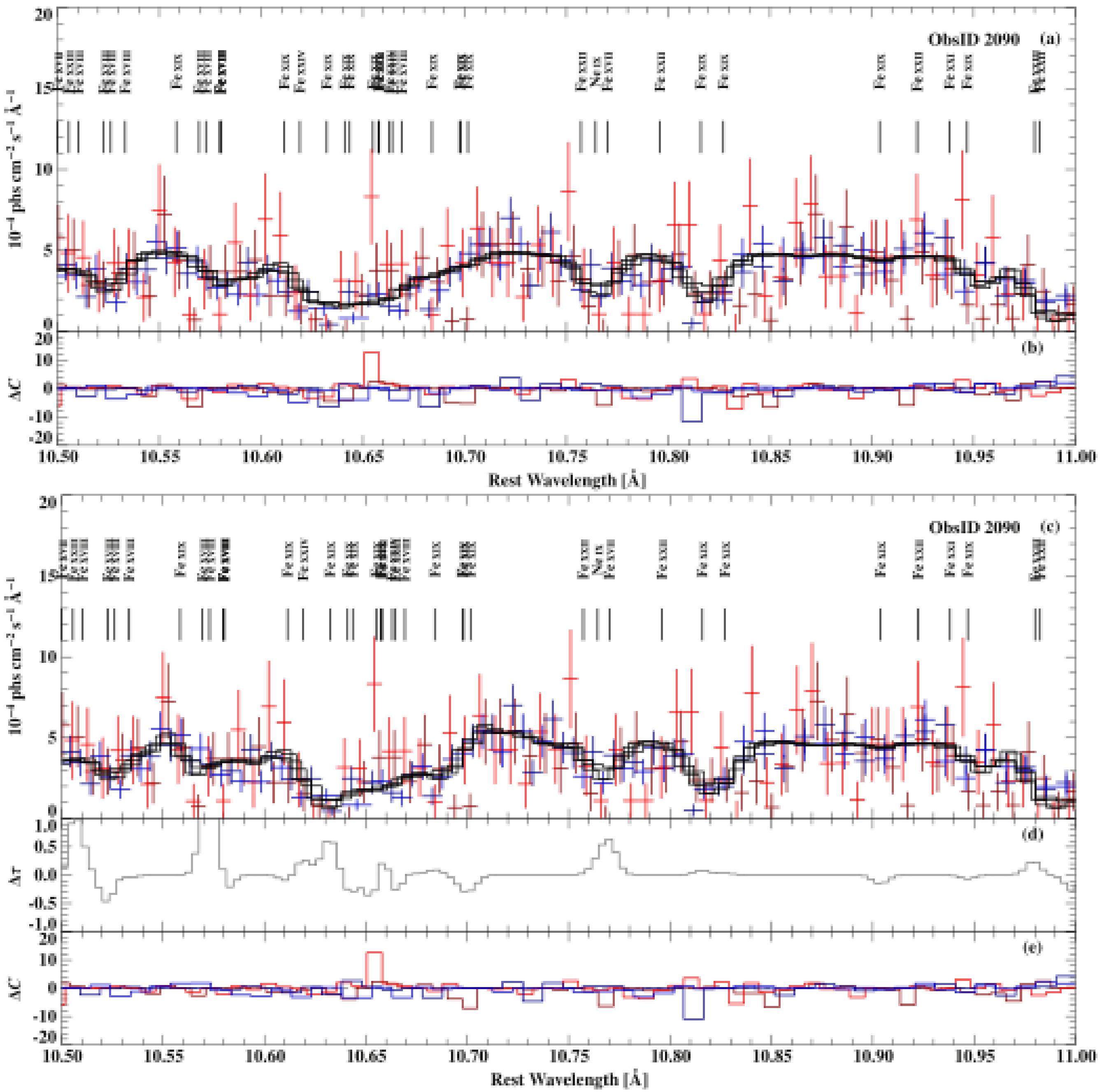
Atomic data Accuracy: the HETG spectrum of NGC 3783

Best fit, 5 components each with ~2000 known lines
C_{stat}=47254.0/41698=1.13

Why don't we get a perfect fit?

Additional absorption by known lines with added ad hoc additional optical depth
C_{stat}=45250.2/41251=1.09

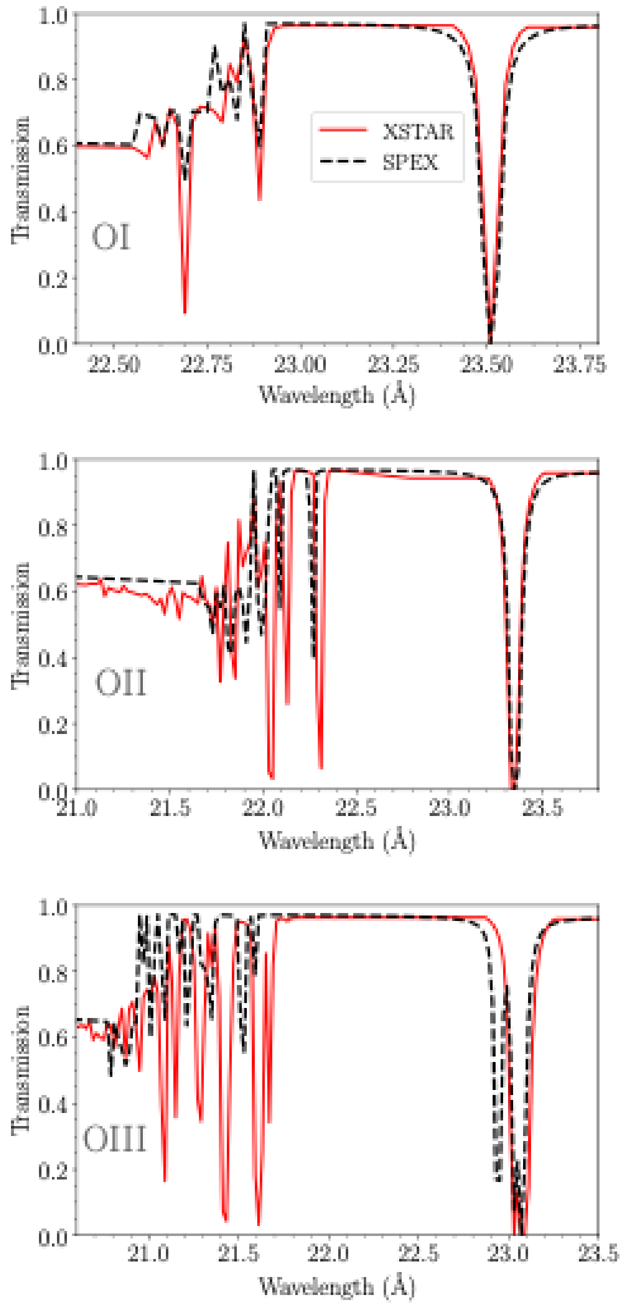
→ *It appears that errors in absorption line strengths is not the primary reason for C_{stat}/ν>1*



Ballhausen et al 2023

Atomic data accuracy: Comparing codes is a useful check

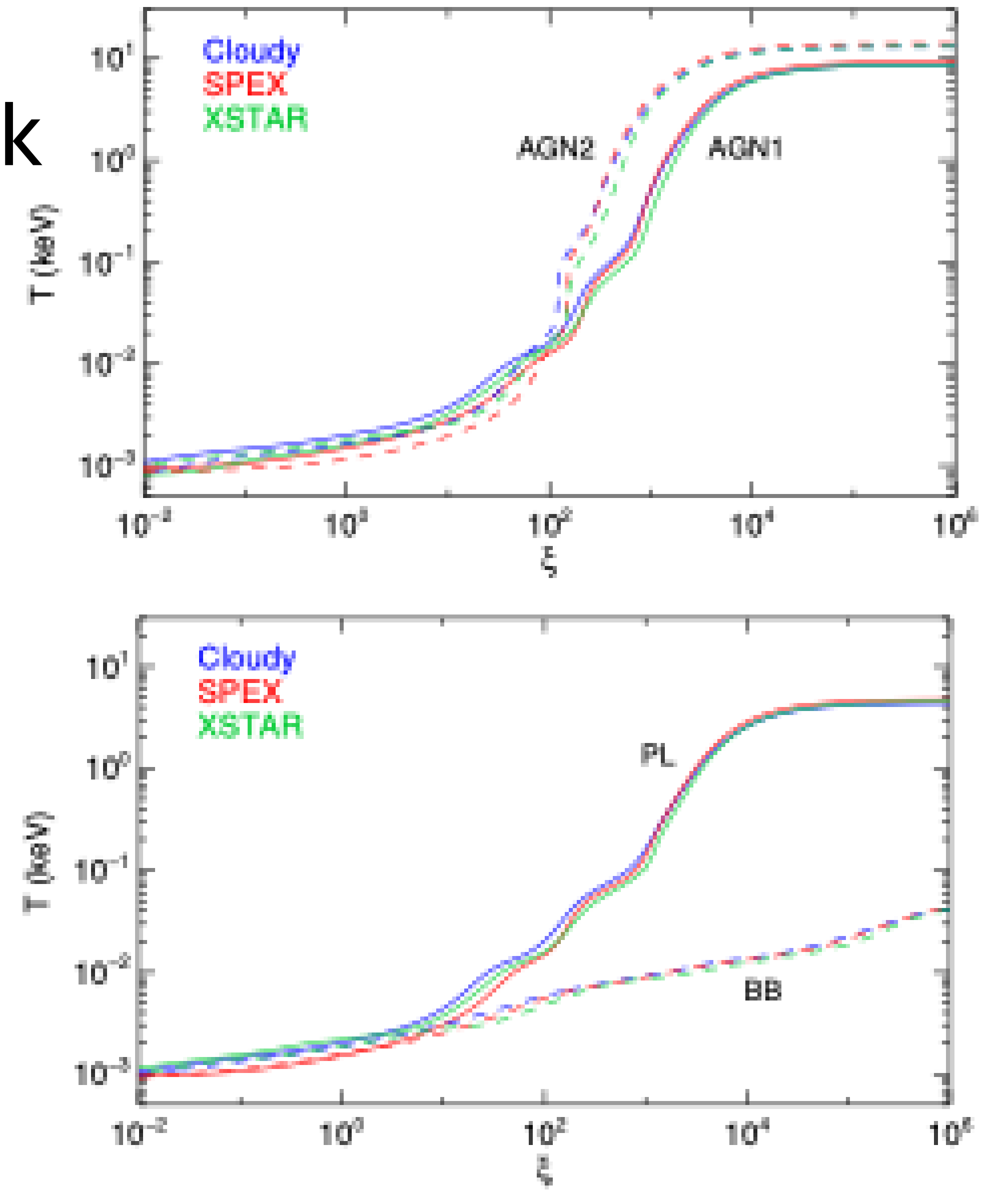
- Recent comparison of predictions at the OI K edge shows agreement on gross features.
- Location of individual resonances differs by Δe/e~0.001 in some cases
- Consistent with expectation but not adequate for high s/n work.



(Psaradaki et al. 2020)

Atomic data accuracy:
Comparing codes is a useful check

- Comparison of temperature produced by various photoionization codes
- Shows very good agreement for this particular problem.

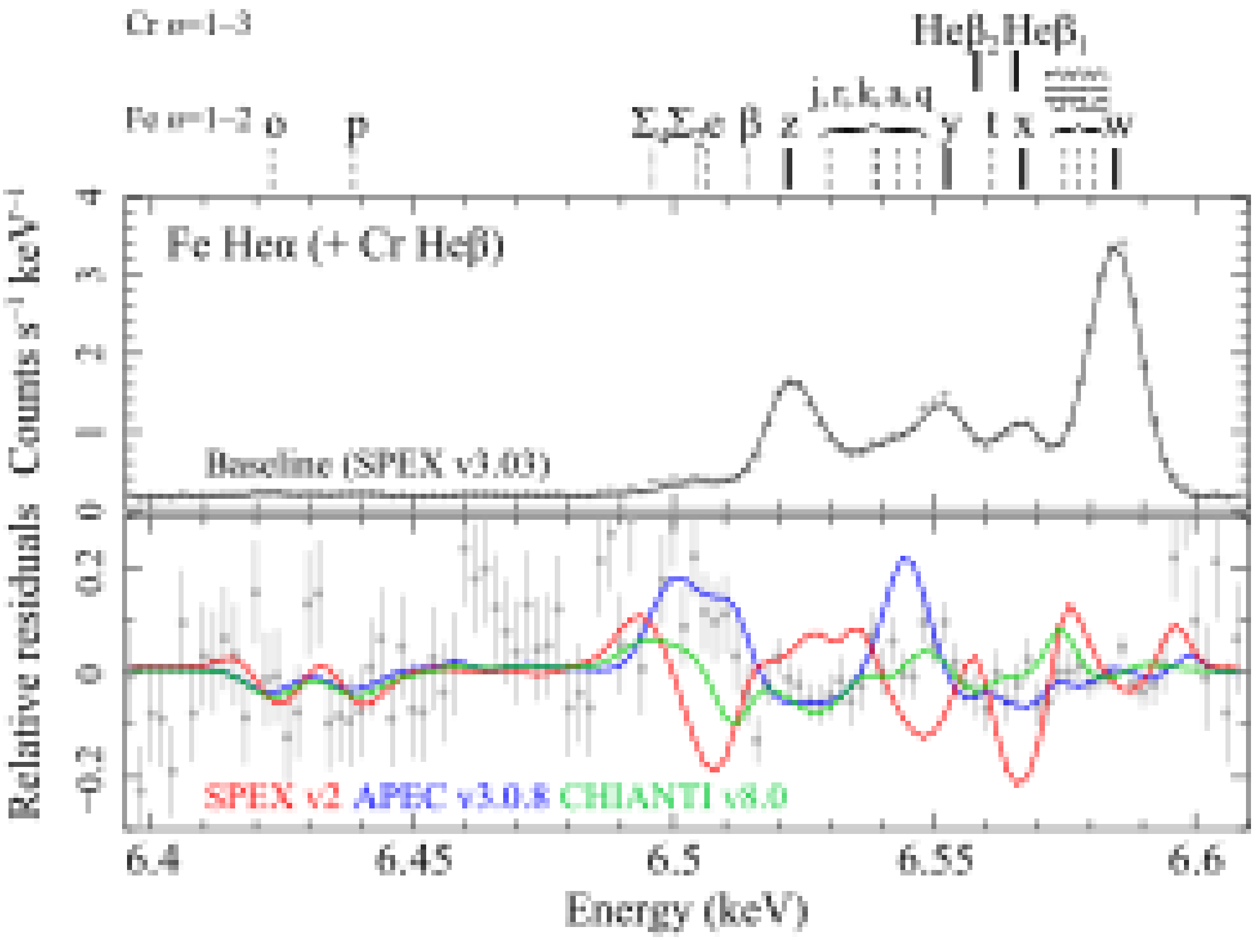


(Mehdipour et al. 2016)

Atomic data accuracy: Comparing codes is a useful check

Hitomi Perseus spectrum:

- Various code predictions are compared
- Final spectrum shows good consistency
- Residuals from different codes show larger differences, particularly in the Fe XXIV region

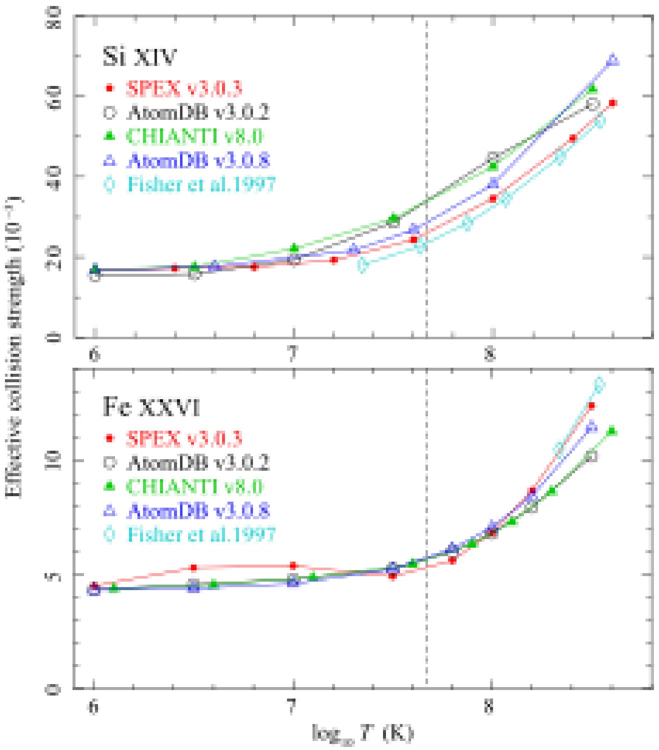


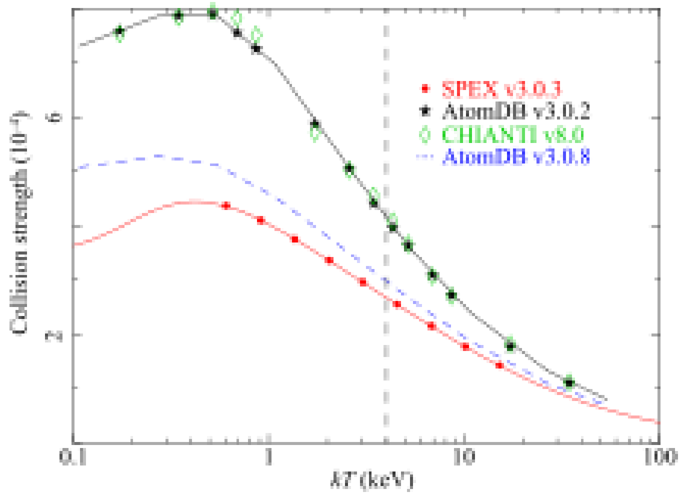
(Hitomi et al. 2018)

Atomic data accuracy: Comparing codes is a useful check

Hitomi Perseus spectrum:

- Various sources for electron impact collisional excitation are compared
- Strongest transitions show good consistency
- Forbidden transitions are less secure
- Lower value for 1s2-2s2p($^3S_1$) produces models which fit data better





(Hitomi et al. 2018)

Atomic data accuracy:
Experimental validation of results

PRL 119, 075001 (2017) PHYSICAL REVIEW LETTERS week ending 18 AUGUST 2017

Benchmark Experiment for Photoionized Plasma Emission from Accretion-Powered X-Ray Sources

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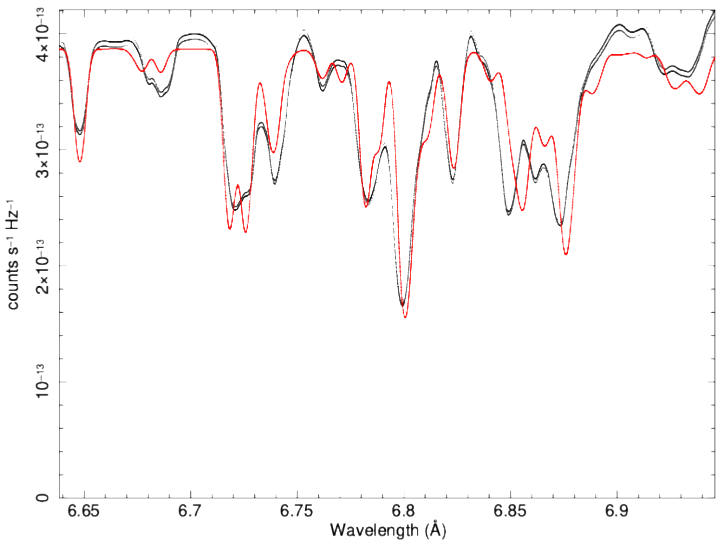
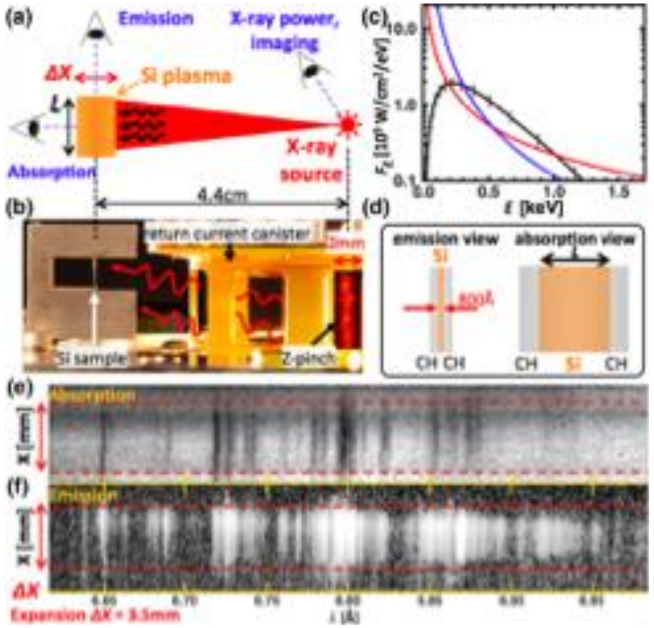
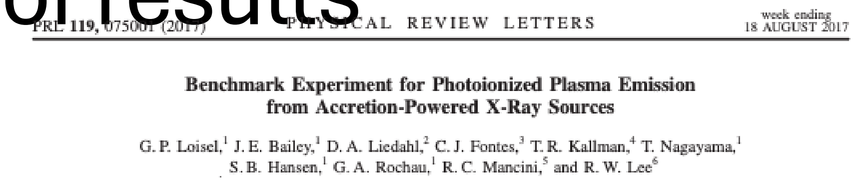
- Code results (xstar) have been compared with experiment which produces a photoionized plasma in the lab
- Pure Si at log(ξ)~2
- Qualitative agreement is found for absorption spectrum





Atomic data accuracy:
Experimental validation of results



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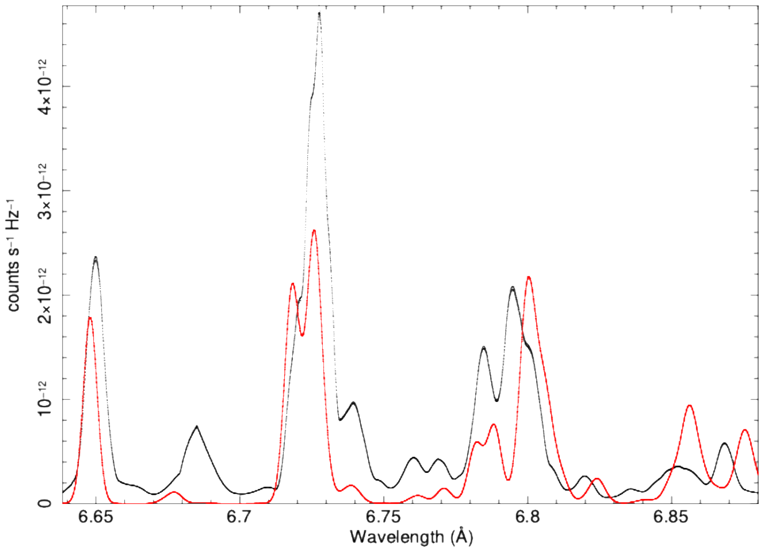
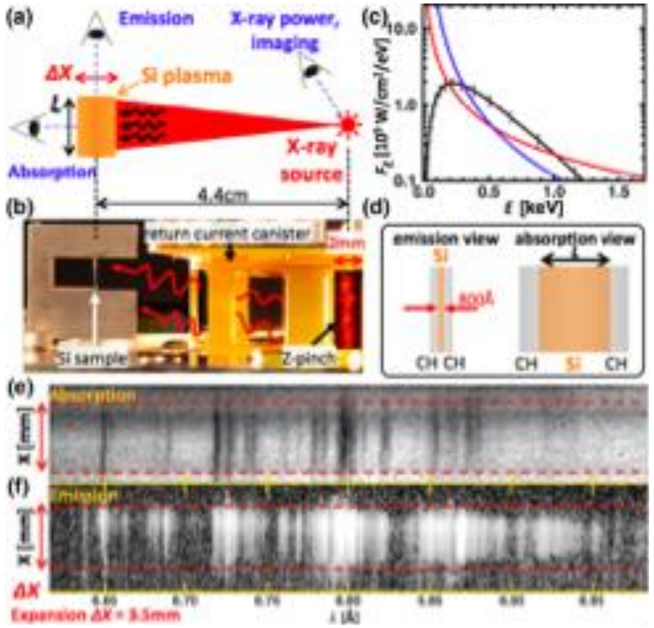
- Code results (xstar) have been compared with experiment which produces a photoionized plasma in the lab
- Pure Si at log(ξ)~2
- Qualitative agreement is found for absorption spectrum
- Less good fit for emission → radiative transfer effects?





Atomic data accuracy: More about atomic data

- Newer does not necessarily imply more accurate
- Many energies depend on calculations
- Careful about damping
- Neutral atoms and near-neutrals are the frontier
- Rates affecting K shells of heavies are challenging computationally

Models can be affected by ` unknown unknowns':

- Departures from equilibrium (Time dependence)
- complicated (non-spherical or plane parallel) geometry
- Dynamical (i.e. departures from simple description involving turbulence and radial flow)
- Non-Maxwellian electrons
- Relativistic particles
- Extra neutrals → charge exchange

- But this is interesting, this is where the science is…

How accurate is the assumption of ionization equilibrium?

$$t_{rec} = \frac{1}{n_e \alpha_{rec}(T)} \sim \frac{10^{11}\mathrm{s}}{n_e}$$

$$t_{ion} = \frac{1}{\int_{\varepsilon_{Th}}^{\infty} F_\varepsilon \sigma_{PI}(\varepsilon) d\varepsilon/\varepsilon} \sim \frac{10^{7}\mathrm{s}}{n_e \xi}$$

$$t_{decay} = \frac{1}{A_{ul}} \sim 10^{-10}\mathrm{s}$$

- Processes which occur on timescales shorter than these will drive the gas out of equilibrium
- Examples include:
  - Changes in ionizing flux
  - Changes in gas density (eg. Due to gas motions)

Summary

- Models are necessary for analyzing high resolution X-ray spectra
- Modeling requires large database of atomic rate data
- And relatively simple assumptions
- Various modeling packages exist
- Care is needed when interpreting model results, particularly when discovering something new

Resources

- ‘Astrophysics of Gaseous Nebulae’ Osterbrock and Ferland
- A. K. Pradhan & S. N. Nahar, “Atomic Astrophysics and Spectro-scpy”, Cambridge University Press (2011)
- http://heasarc.gsfc.nasa.gov/xstar.html