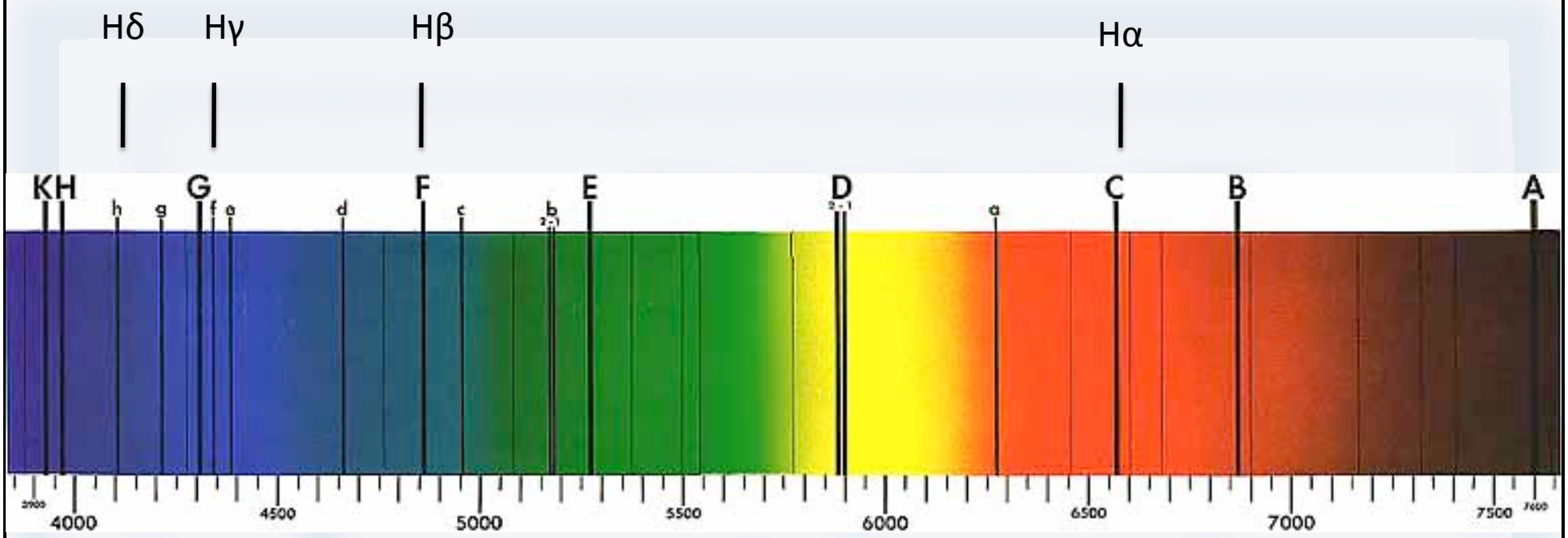
BASICS OF SPECTROSCOPY

Spectroscopy School,
MSSL, March 17-18, 2009

Frits Paerels
Columbia Astrophysics Laboratory
Columbia University, New York

cgs units throughout!



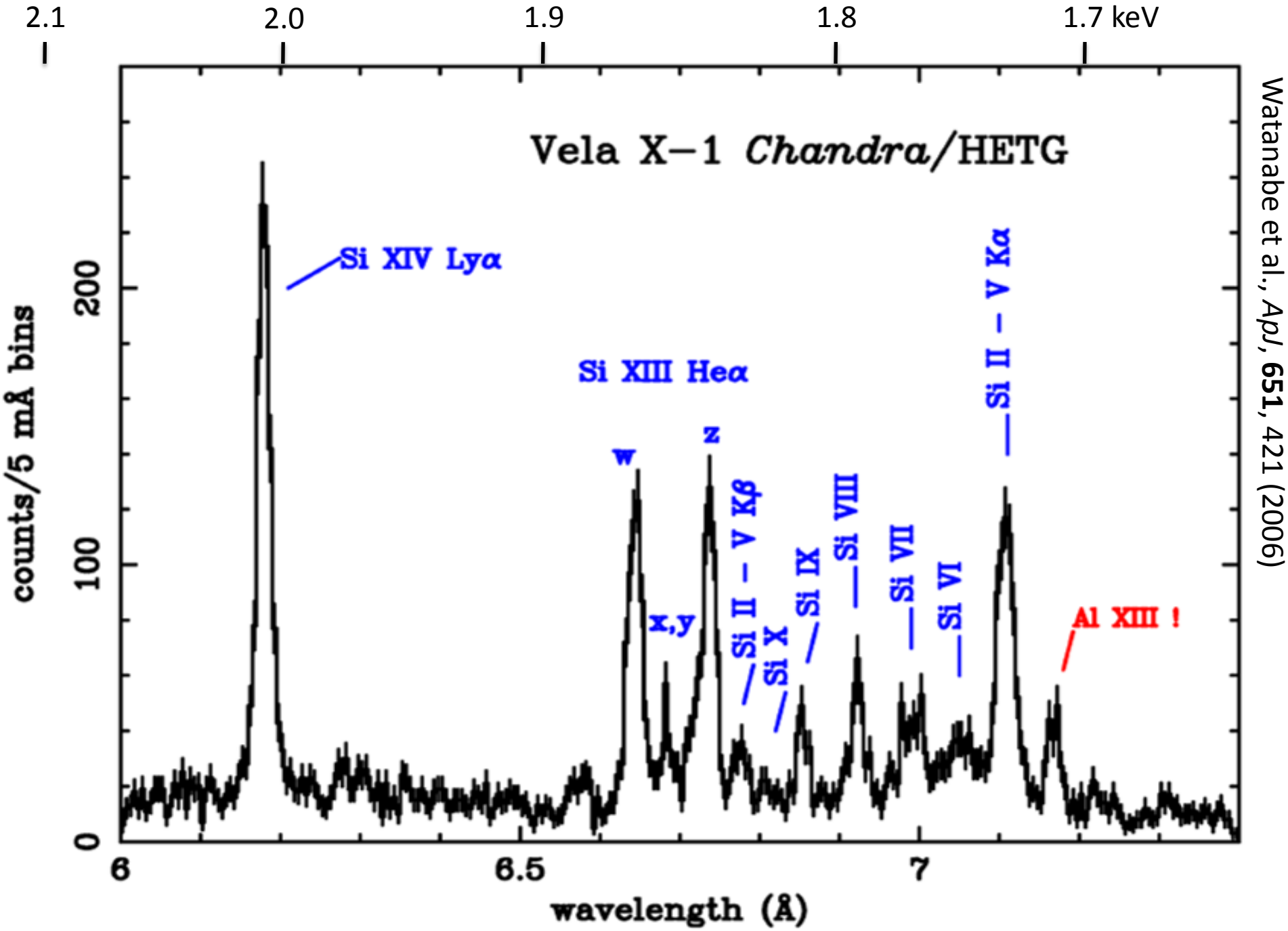
Wavelength (Å)

NB: 1 Å = 10^{-8} cm

E = hc/λ: E(keV) = 12.3985/λ(Å)

Astrophysical X-ray band: 0.1-100 keV (> 10 keV 'hard X-rays', no atomic spectroscopy)

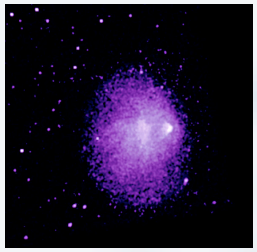
0.1-10 keV corresponds to ~1-100 Å

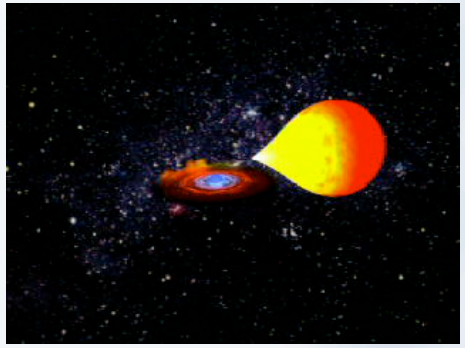


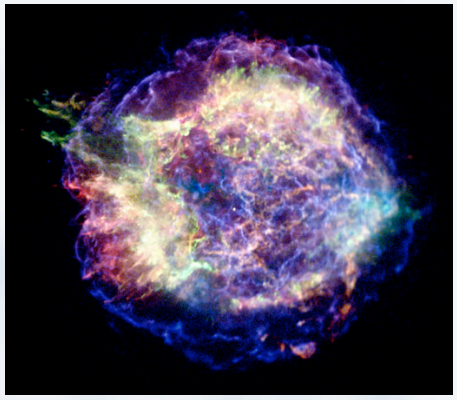
Watanabe et al., *ApJ*, **651**, 421 (2006)

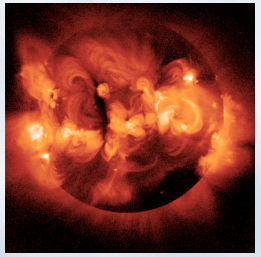
Spectrum provides precise information on 'local' conditions in the plasma

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



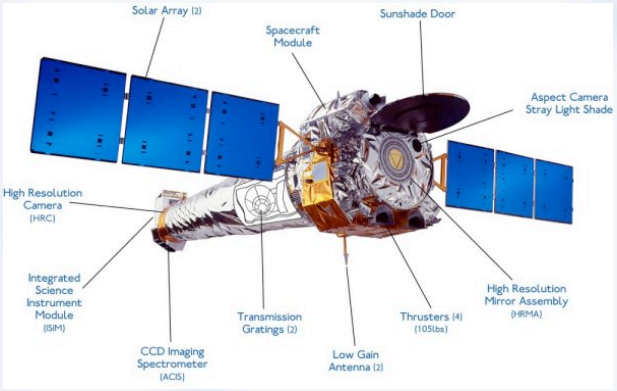






In this talk, I will concentrate on the basics: how, what, why of the spectrum-
before you attempt some sort of 'global fit' or 'model fit'

For Reference: Current Instrumentation



Chandra X-ray Observatory

HETGS (High Energy Transmission Grating Spectrometer)

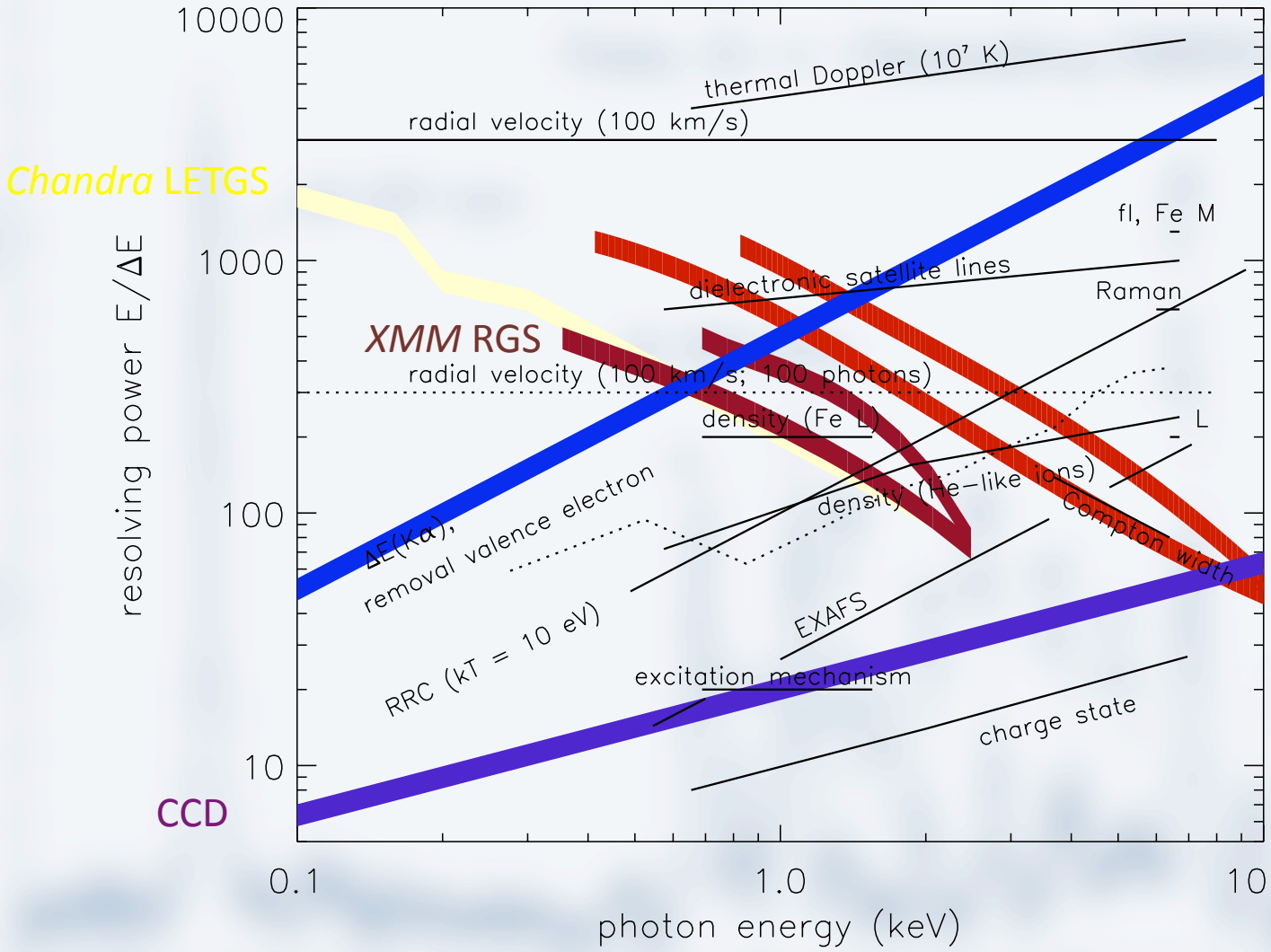
LETGS (Low Energy Transmission Gr…)

XMM-Newton

RGS (Reflection Grating Spectrometer)

and CCD spectrometers on *Chandra*, *XMM-Newton*, *Suzaku*, and *Swift*

Resolving Power



Chandra LETGS

CCD

ΔE = 2 eV Micro-calorimeter

Chandra HETGS

‘real’ spectroscopy only since 2000
(*Chandra* and *XMM* diffraction grating spectrometers)

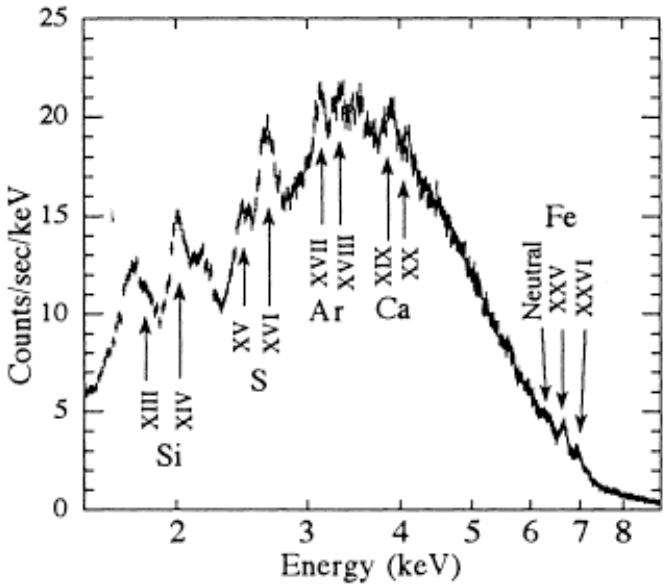
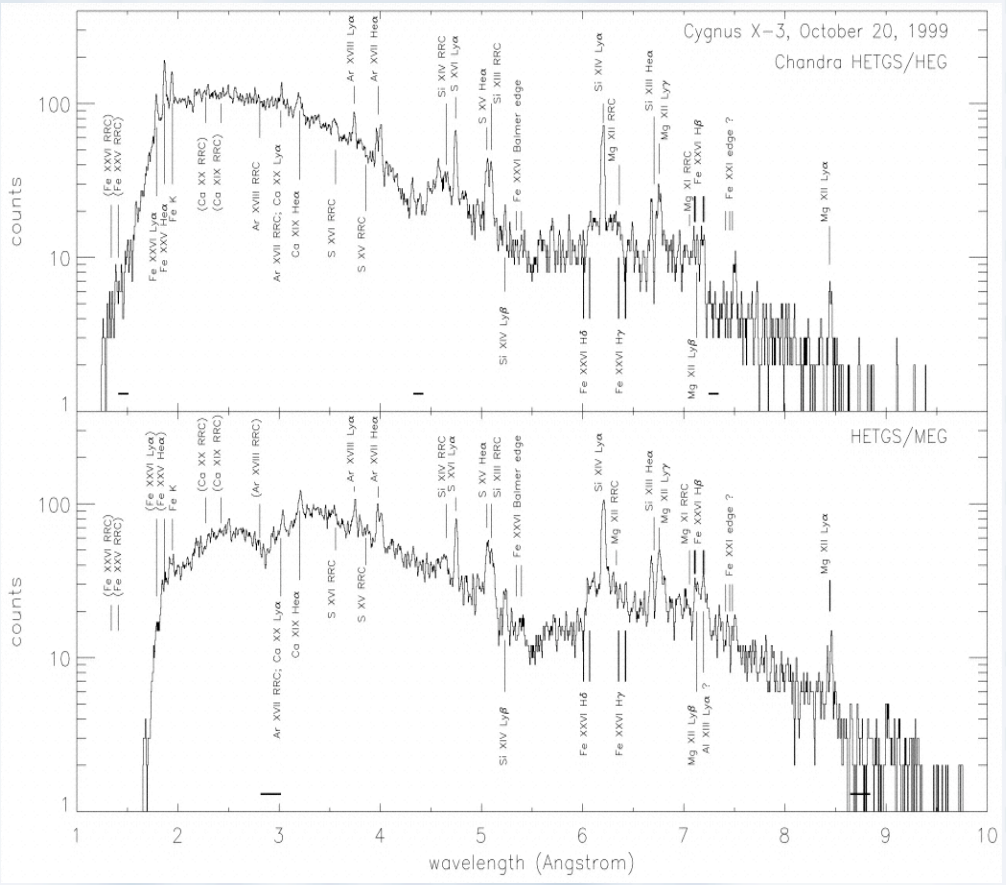


Fig. 1. Energy spectrum of Cyg X-3 obtained by SIS. Identifications for prominent lines are also indicated by arrows.

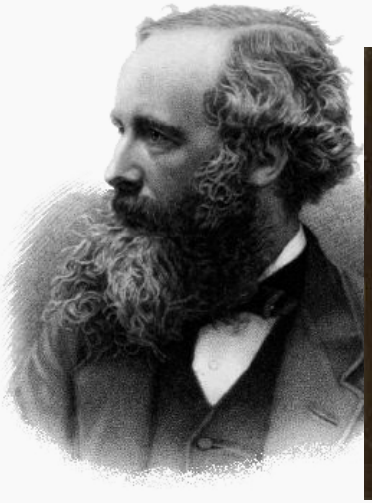
Kitamoto et al. (1994)



Paerels et al. (2000)

Cygnus X-3 with *ASCA* CCDs and *Chandra* HETGS

WAVELENGTH OR PHOTON ENERGY ?

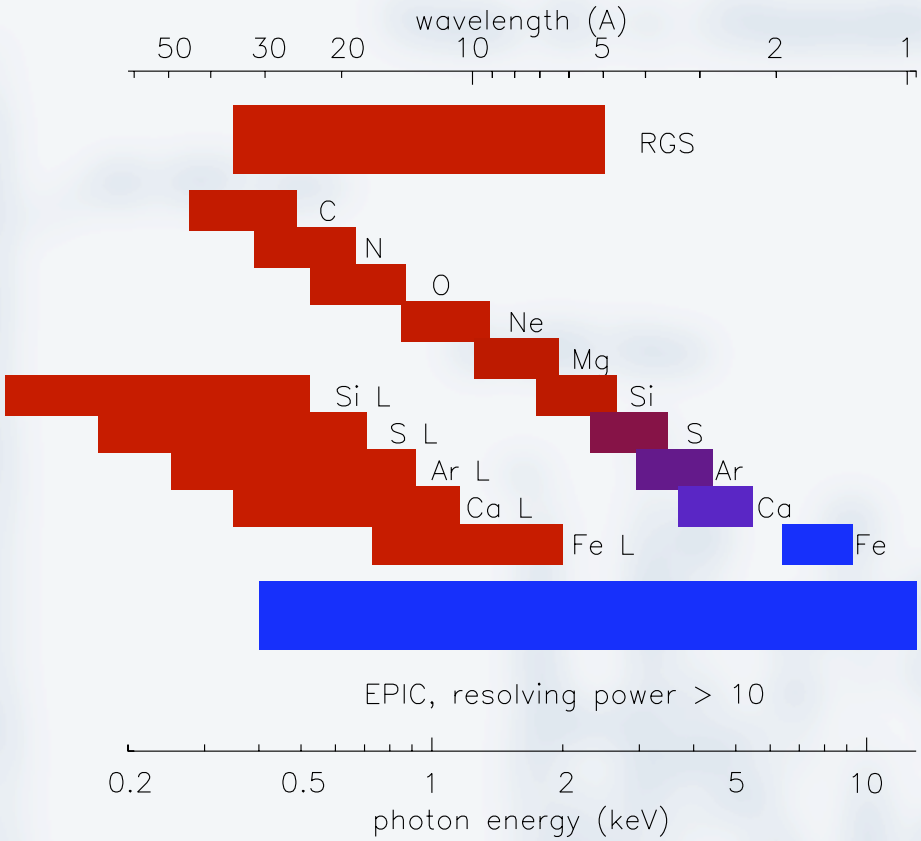


Diffraction gratings: $\Delta\lambda$ constant

Ionization detectors, calorimeters: ΔE constant or slow function of E

(see tomorrow's lecture)

Detection and Identification



X-ray spectra, between neutral fluorescent n=2-1, and H-like n=1-∞

Never leave home without the Bohr model!

Detection and Identification: What are you looking at?
Atomic Structure, energy levels

H-like ions:

$$E_n = \frac{-Z^2\mathcal{R}}{n^2} \Rightarrow$$

$$\frac{E_n}{m_e c^2} \sim \mathcal{O}\left(\frac{v^2}{c^2}\right) = -\frac{1}{2}\alpha^2\frac{Z^2}{n^2}$$

$$\frac{E_n}{m_e c^2} > 10^{-3} \Rightarrow Z > 6!!$$

(Z: nuclear charge; $\mathcal{R}$: Rydberg, 13.6 eV; $\alpha = 1/137$)

10^{-3} is not small: at 20 Å, $\Delta\lambda = 0.02$ Å !

Also, $v = 10^{-3}\, c = 300$ km/s

So we need the relativistically correct equations: Dirac equation
(at least; if not QED)

Detection and Identification: What are you looking at?
Atomic Structure, energy levels

$$\frac{E_n}{m_e c^2} = \left\{1 + \left(\frac{\alpha Z}{n - k + \sqrt{k^2 - \alpha^2 Z^2}}\right)^2\right\}^{-1/2} - 1$$

$$E_n \approx \frac{-Z^2 \mathcal{R}}{n^2}\left\{1 + \frac{(\alpha Z)^2}{n}\left(\frac{1}{k} - \frac{3}{4n}\right)\right\}$$

n = 1, 2, 3, …
k = 1, 2, …, n

(careful if the 'fine structure' (k) components of a line are not resolved by your spectrometer- you measure the weighted wavelength of the two components)

Transitions should properly be called Lyα,β,γ,…, Hα,β,…

Bethe and Salpeter*: the Quantum Mechanics of One-and Two-Electron Atoms*

Term symbol

From Wikipedia, the free encyclopedia

In quantum mechanics, the **term symbol** is an abbreviated description of the angular momentum quantum numbers in a multi-electron atom. It is related with the energy level of a given electron configuration. LS coupling is assumed. The ground state term symbol is predicted by Hund's rules.

The term symbol has the form

$$^{2S+1}L_J$$

where

S is the total spin quantum number. 2*S*+1 is the **spin multiplicity**: the maximum number of different possible states of *J* for a given (*L*,*S*) combination.

L is the total orbital quantum number in spectroscopic notation. The symbols for L = 0,1,2,3,4,5 are S,P,D,F,G,H respectively.

J is the total angular momentum quantum number.

When used to describe electron states in an atom, the term symbol usually follows the electron configuration, e.g., in the case of carbon, the ground state is $1s^2 2s^2 2p^2\ ^3P_0$. The 3 indicates that 2S+1=3 and so S=1, the P is spectroscopic notation for L=1, and 0 is the value of J.

LS coupling

[edit]

In light atoms (generally Z<30), electron spins $\mathbf{s}_i$ interact among themselves so they combine to form a total spin angular momentum **S**. The same happens with orbital angular momenta $\mathbf{l}_i$, forming a single orbital angular momentum **L**. The interaction between the quantum numbers **L** and **S** is called **Russell-Saunders coupling** or **LS coupling**. Then **S** and **L** add together and form a total angular momentum **J**:

$$\mathbf{J} = \mathbf{L} + \mathbf{S}, \text{ where}$$
$$\mathbf{L} = \sum_i \mathbf{l}_i \text{ and}$$
$$\mathbf{S} = \sum_i \mathbf{s}_i.$$

Detection and Identification

He-like ions:

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'**

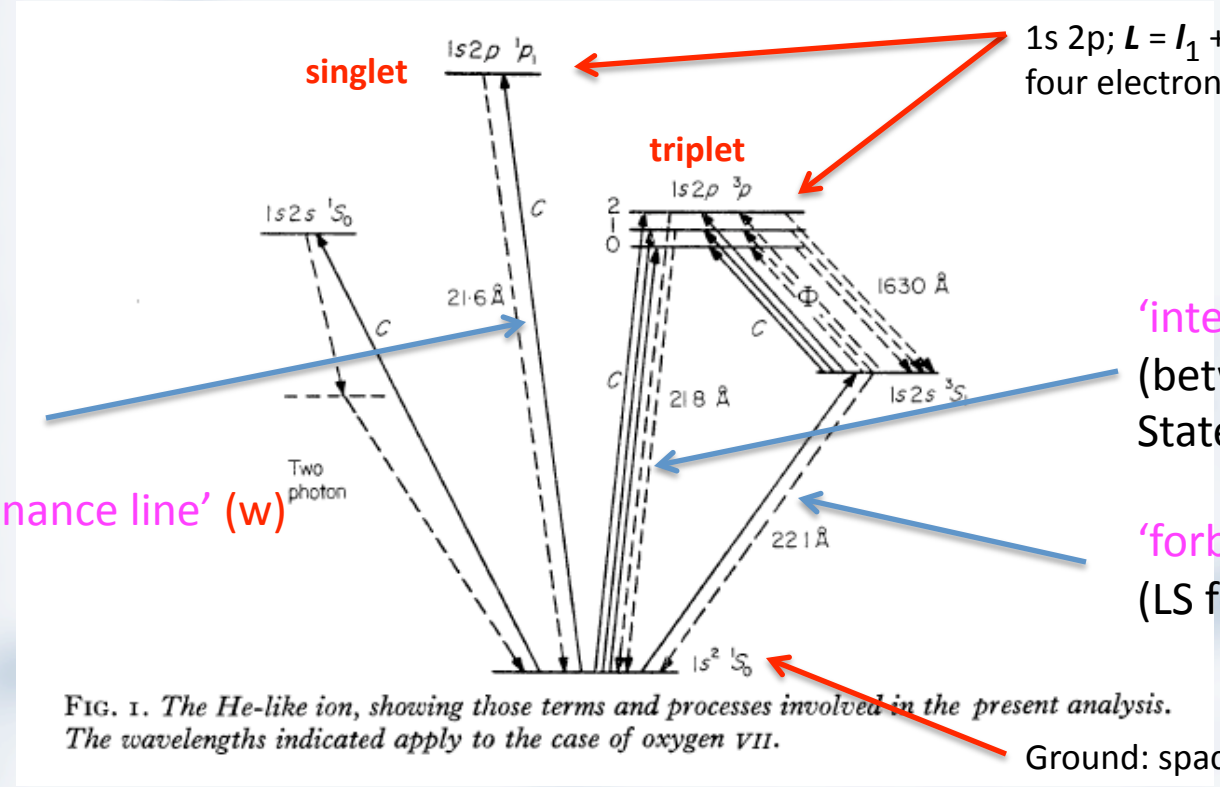


FIG. 1. *The He-like ion, showing those terms and processes involved in the present analysis. The wavelengths indicated apply to the case of oxygen VII.*

1s 2p; $\boldsymbol{L} = \boldsymbol{l}_1 + \boldsymbol{l}_2 = 1$, 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

H- and He-like ions in practice: wavelengths

Courtesy Masao Sako, University of Pennsylvania

H-LIKE SPECIES

Ion	Lyα_1		Lyα_2		K-edge	
	λ (Å)	E (keV)	λ (Å)	E (keV)	λ (Å)	E (keV)
C VI	33.7342	0.36754	33.7396	0.36747	25.3033	0.489993
N VII	24.7792	0.50036	24.7846	0.50024	18.5871	0.667046
O VIII	18.9671	0.65368	18.9725	0.65348	14.2280	0.871410
Ne X	12.1321	1.02195	12.1375	1.02150	9.10177	1.36220
Na XI	10.0232	1.23697	10.0286	1.23631	7.52011	1.64870
Mg XII	8.41920	1.47264	8.42461	1.47169	6.31714	1.96266
Al XIII	7.17091	1.72899	7.17632	1.72769	5.38093	2.30414
Si XIV	6.18043	2.00608	6.18584	2.00432	4.63808	2.67318
S XVI	4.72735	2.62270	4.73276	2.61970	3.54830	3.49419
Ar XVIII	3.73110	3.32299	3.73652	3.31817	2.80113	4.42622
Ca XX	3.01848	4.10750	3.02390	4.10014	2.26668	5.46986
Fe XXVI	1.77802	6.97316	1.78344	6.95197	1.33637	9.27769

Lines: Johnson, W. R., & Soff, G. 1985, Atom. Data Nucl. Data Tables, **33**, 405

HE-LIKE SPECIES

Ion	w(resonance)		x(intercombo)		y(intercombo)		z(forbidden)		K-edge	
	λ (Å)	E (keV)	λ (Å)	E (keV)	λ (Å)	E (keV)	λ (Å)	E (keV)	λ (Å)	E (keV)
C V	40.2674	0.307902	40.7280	0.304420	40.7302	0.304404	41.4718	0.298960	31.63	0.392
N VI	28.7800	0.430800	29.0819	0.426328	29.0843	0.426293	29.5346	0.419793	22.46	0.552
O VII	21.6015	0.573961	21.8010	0.568709	21.8036	0.568641	22.0974	0.561080	16.78	0.739
Ne IX	13.4473	0.922001	13.5503	0.914992	13.5531	0.914803	13.6984	0.905100	10.37	1.196
Na X	11.0029	1.12683	11.0802	1.11897	11.0832	1.11867	11.1918	1.10781	8.463	1.465
Mg XI	9.16875	1.35225	9.22817	1.34354	9.23121	1.34310	9.31362	1.33121	7.037	1.762
Al XII	7.75730	1.59829	7.80384	1.58876	7.80696	1.58812	7.87212	1.57498	5.944	2.086
Si XIII	6.64795	1.86500	6.68499	1.85467	6.68819	1.85378	6.73949	1.83967	5.085	2.438
S XV	5.03873	2.46062	5.06314	2.44876	5.06649	2.44714	5.10067	2.43074	3.846	3.224
Ar XVII	3.94907	3.13958	3.96587	3.12628	3.96936	3.12353	3.99415	3.10414	3.009	4.121
Ca XIX	3.17715	3.90237	3.18910	3.88775	3.19275	3.88330	3.21103	3.86120	2.417	5.129
Fe XXV	1.85040	6.70040	1.85541	6.68231	1.85952	6.66754	1.86819	6.63659	1.404	8.828

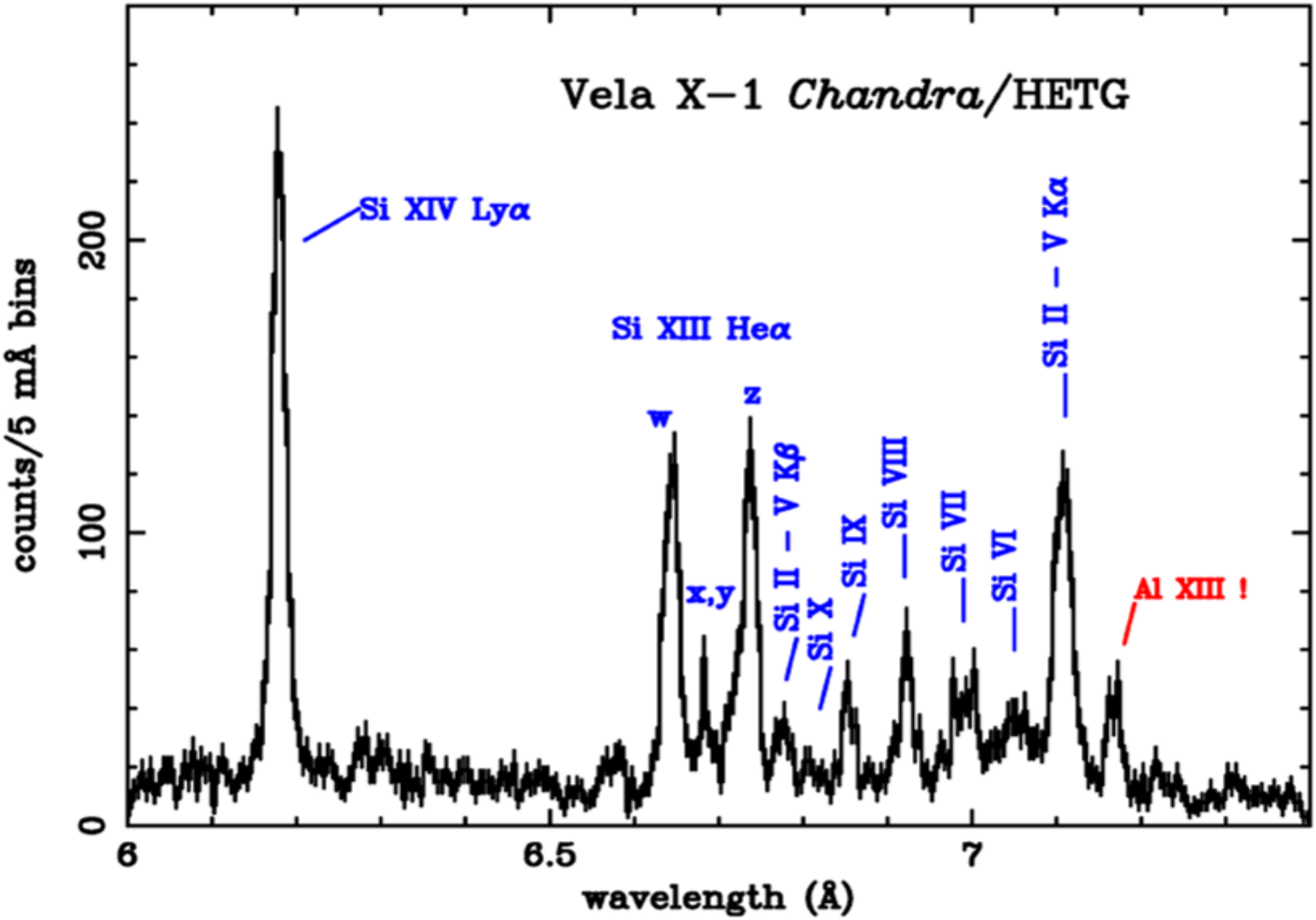
Lines: Drake, G. W. 1988, Can. J. Phys., **66**, 586
Edges: HULLAC, except for Na & Al (Verner et al. 1996, ApJ, **465**, 487)

Calculate structure of multi-electron ions: e.g.

HULLAC (Hebrew Univ. LLNL Atomic Code), M. Klapisch et al.,2007, *AIP Conf. Proc.*, **926**, 206

FAC (Flexible Atomic Code), M. F. Gu,2003, *ApJ*, **582**, 1241 *and lots of experimental work!*

Li-like ions, and below: Fluorescence



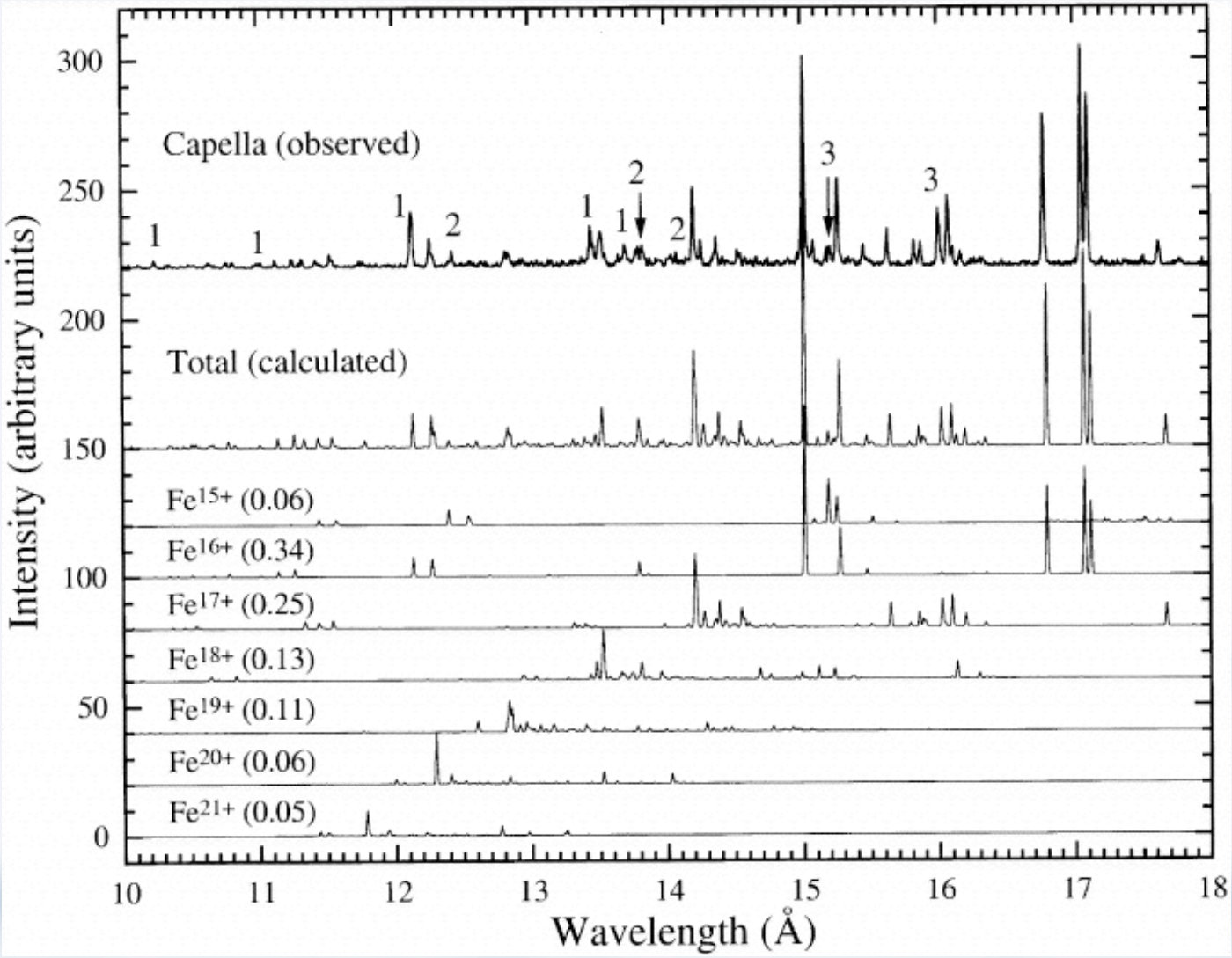
Watanabe et al., *ApJ*, **651**, 421 (2006)

Fluorescence

- General dependence of line wavelengths on charge state obvious
- all strong transitions for all charge states located in a relatively narrow band (unique to X-ray band!)
- fluorescence can be induced by anything that knocks out innershell electrons (fast electrons, photons, cosmic rays)
- fluorescence yield very strongly dependent on *Z* (0.34 for neutral Fe); light elements don't fluoresce brightly- but in presence of steep ionizing spectrum, can still get comparable fluorescent intensities

- careful with wavelengths: fluorescent photon energy depends on energy of upper level (usually n=2) – sensitive in principle to Ionization (see Vela X-1 spectrum), but also chemical state (molecules, solid compounds). Many lab measurements based on solids!

The Fe L series (electrons in n=2): Li-like to Ne-like (XXIV to XVII)



Capella; *XMM-Newton* RGS; Behar, Cottam, & Kahn, 2001, *ApJ*, **548**, 966

Line strengths

Transition probability, to first order:

$$| < \text{final state} \mid H_{pert} \mid \text{initial state} > |^2$$ (a.k.a. 'Fermi's Golden Rule')

Absorption and emission of radiation:

For H_{pert}, insert interaction of bound electron with external radiation field;

expand the exponential ('multipole expansion');

the final and initial states can be approximated by the stationary states of the unperturbed H (and that brings in the angular momentum and the selection rules)

'permitted, forbidden' transitions

Line strengths

Dipole term: transition rate:

$$A_{n'n} = \frac{2}{3}\frac{e^2\omega^2}{m_e c^3} f \qquad (\text{sec}^{-1})$$

$\omega \sim 1.6 \times 10^{16} Z^2$ Hz (Ly α)

$A_{n'n} \sim 1.6 \times 10^{9} Z^4 f \ \ \text{sec}^{-1}$

f: oscillator strength; for electric dipole n=1-2: f ~ 1; n=1-3: f ~ 0.1

Einstein A, B's

Line strengths

Line flux (or intensity)

Frequently more useful: equivalent width

('contrast' against continuum; extends to absorption spectra; independent of instrumental resolution!)

Emission:

$$EW \equiv \int d\lambda \frac{F_{\rm line} - F_{\rm cont}}{F_{\rm cont}} \quad (\text{Å})$$

$$EW \equiv \int dE \frac{F_{\rm line} - F_{\rm cont}}{F_{\rm cont}} \quad (\text{eV})$$

Easily converted with $d\lambda/\lambda = dE/E = d\nu/\nu = v/c$;

so also quoted as a velocity width

Absorption: flip the signs

Line strengths: absorption

Instructive example: transmission of continuum thru uniform slab

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

Optical depth

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

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

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

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

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

Thermal Doppler width

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

Line strengths: absorption

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

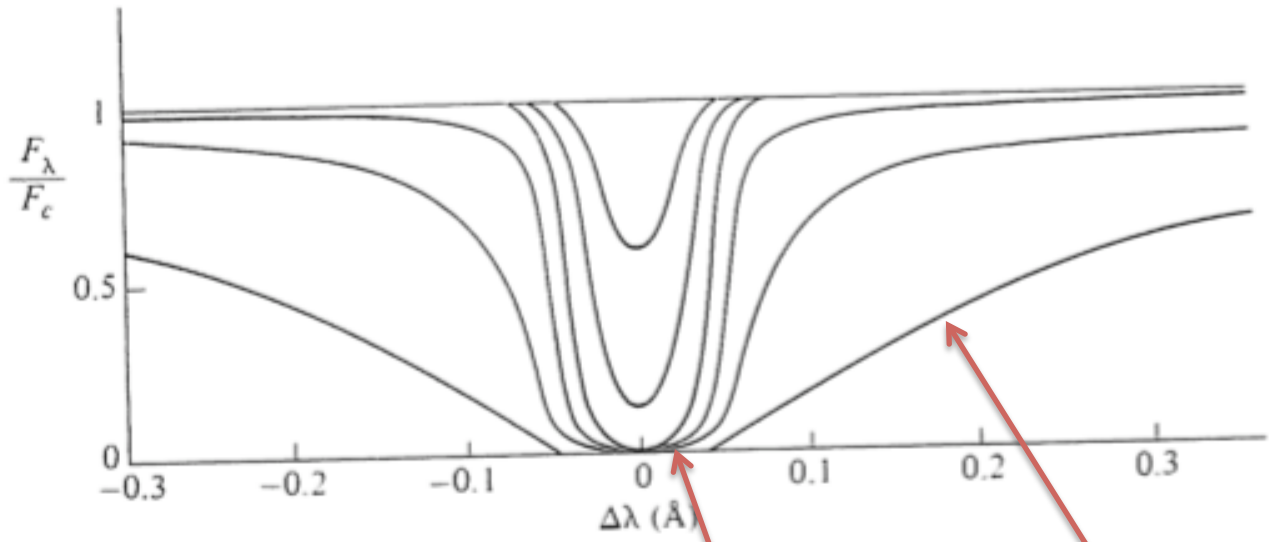


Figure 9.20 Voigt profiles of the K line of Ca II. The shallowest line is produced by $N_a = 3.4 \times 10^{11}$ ions cm^{-2}, and the ions are ten times more abundant for each successively broader line. (Adapted from Novotny, *Introduction to Stellar Atmospheres and Interiors*, Oxford University Press,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

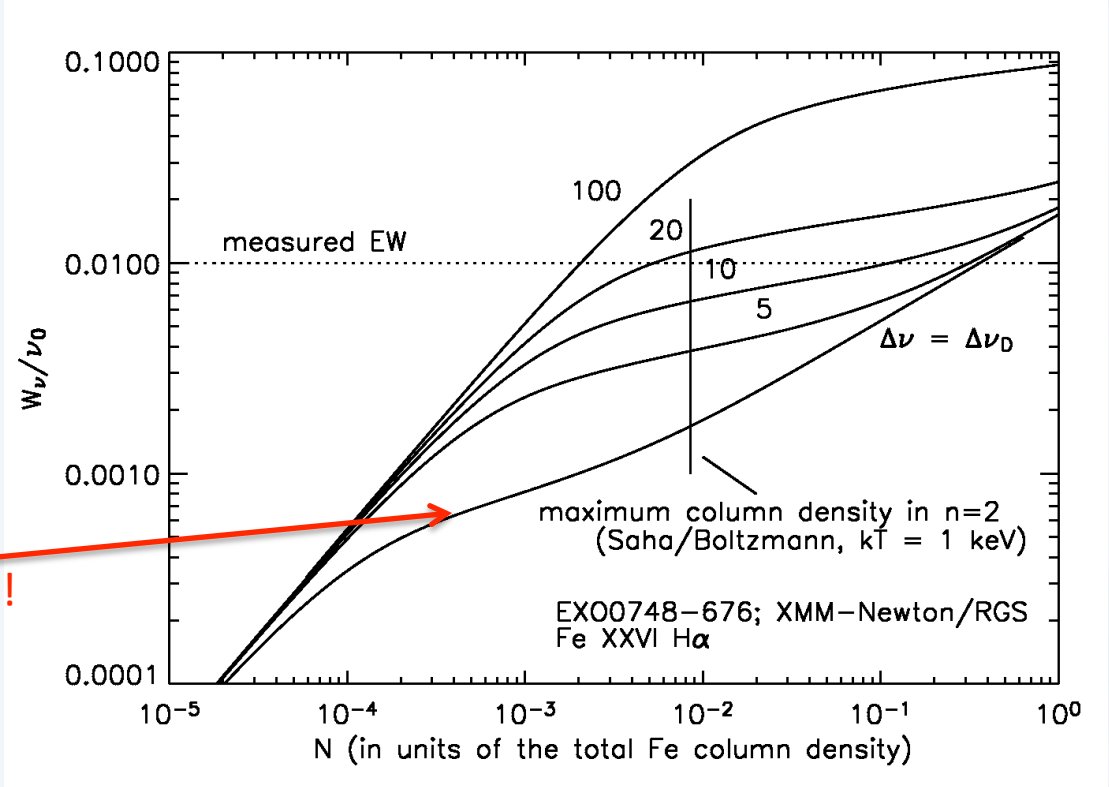
'damping wings'

saturation

From Carroll and Ostlie: Introduction to Modern Astrophysics

Line strengths: absorption

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



Saturation!

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

Detection and Identification:
Spectroscopic Consistency vs. formal significance

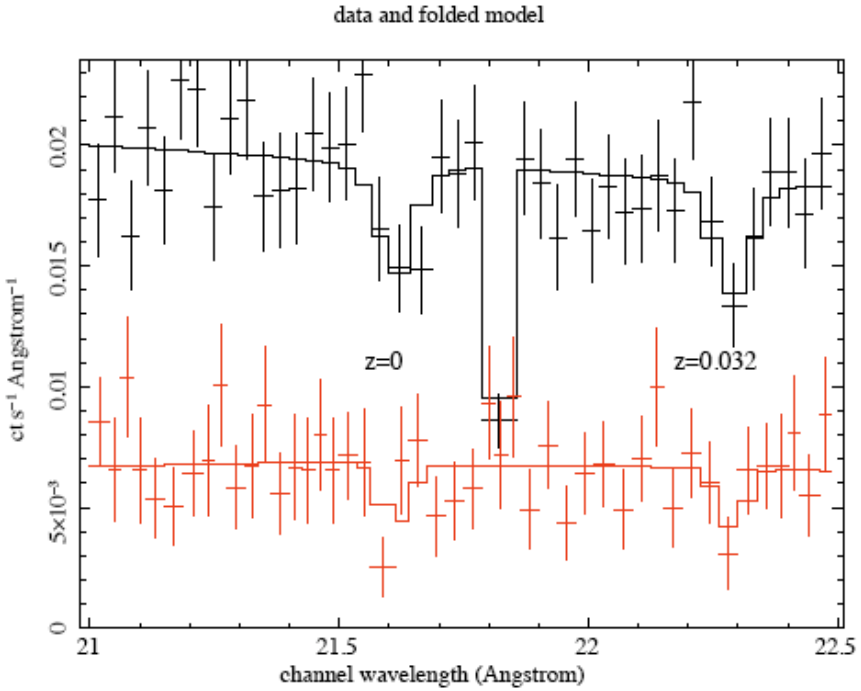


FIG. 2.— Background-subtracted *XMM* (black) and *Chandra* (red) spectra of the blazar H 2356-309 over the wavelength range 21.0−22.5Å used to study the candidate O VII lines. The spectral models represent a power-law continuum, two absorption lines broadened by the instrumental resolution and the Voigt function, and foreground Galactic absorption from cold gas. The wavelength positions of the two absorption lines, nearby and Sculptor, are indicated.

Intergalactic absorption at z = 0.03 (Sculptor Wall) towards H 2356-309

Buote et al., arXiv:0901.380

Case Studies

Interstellar absorption towards X-ray binary Cygnus X-2

(Yao et al., arXiv:0902.2778v1)

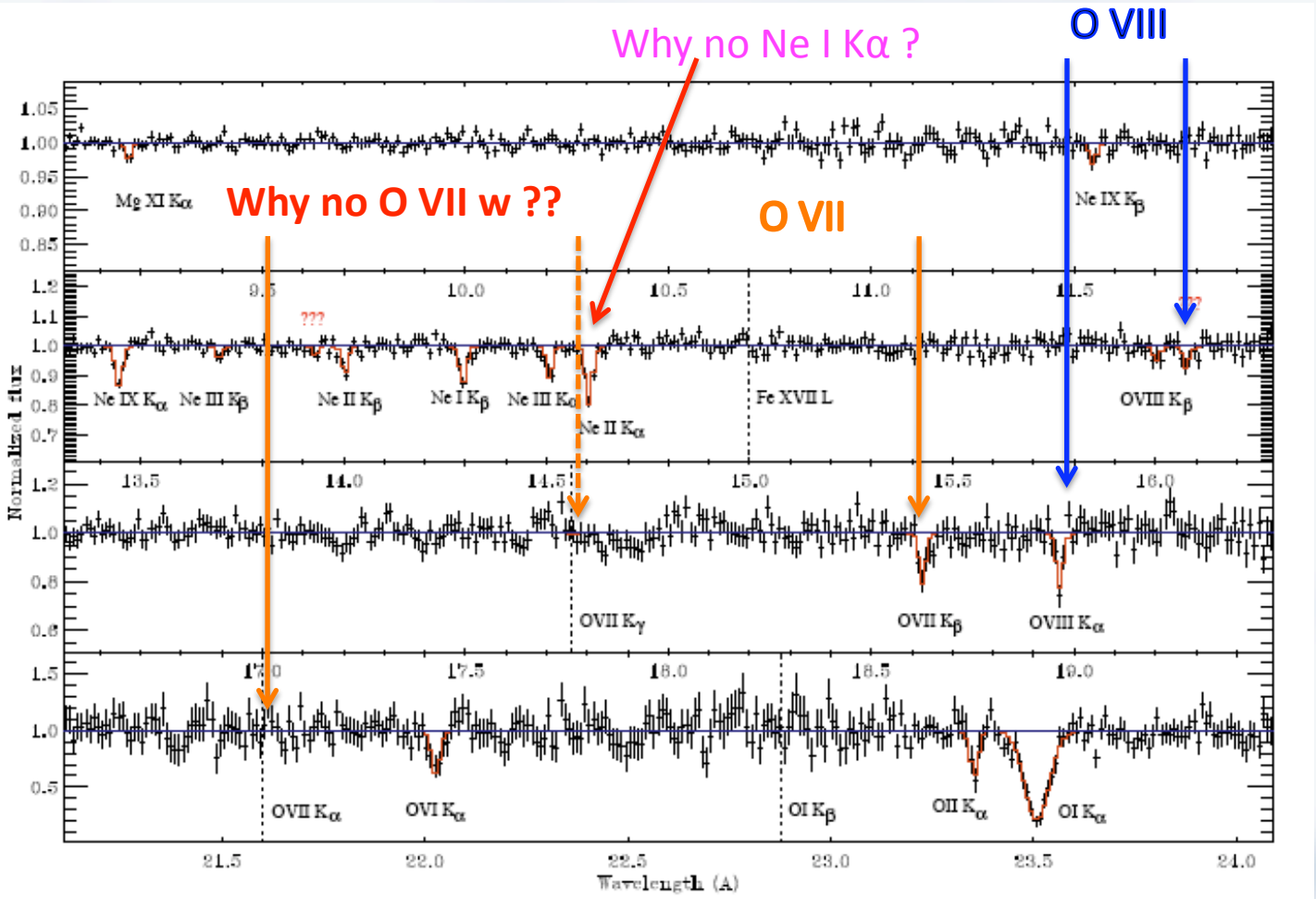


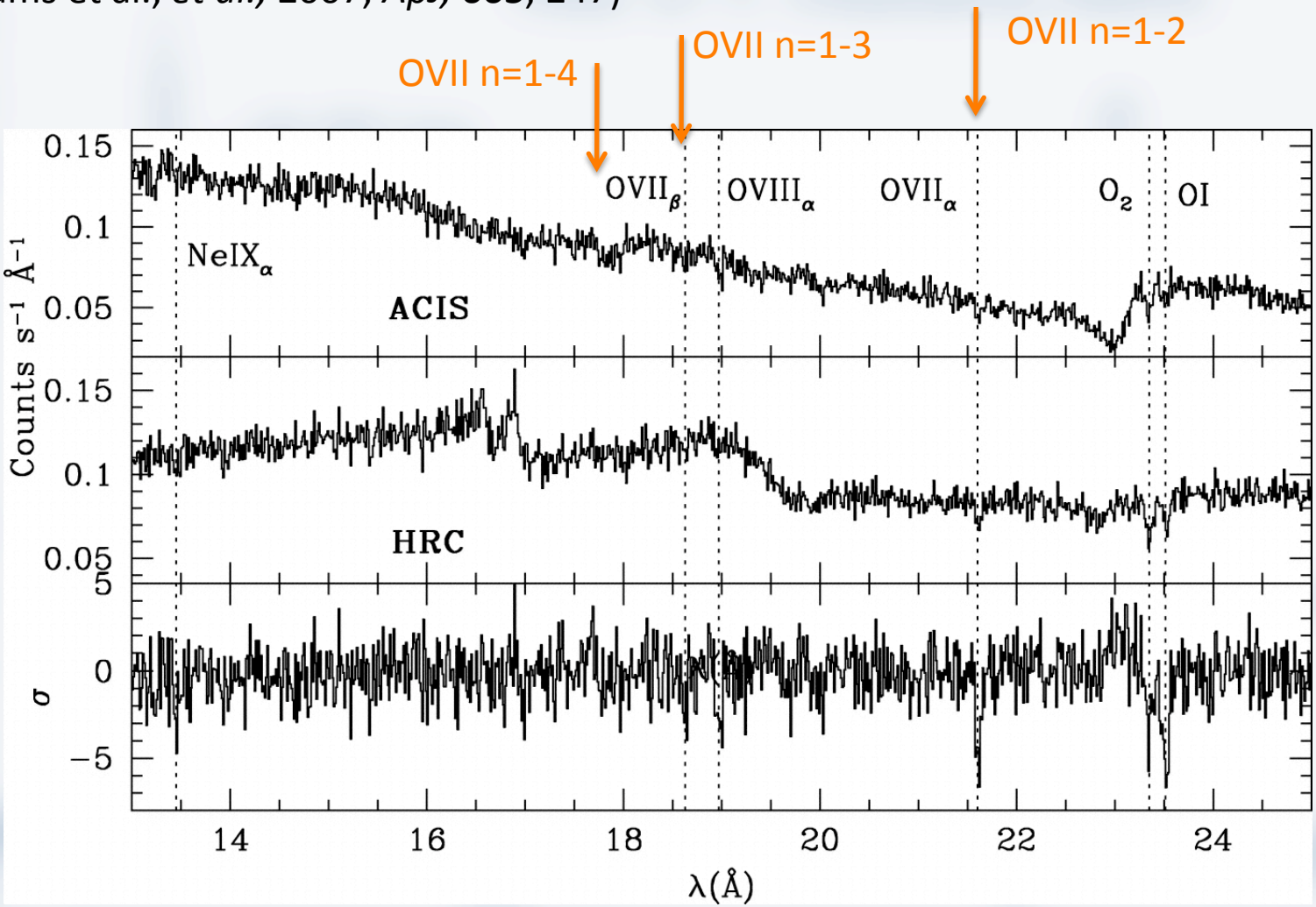
FIG. 2.— Same as the Figure 1, but spectrum is normalized to the best fit continuum.

Chandra HETGS

Case Studies

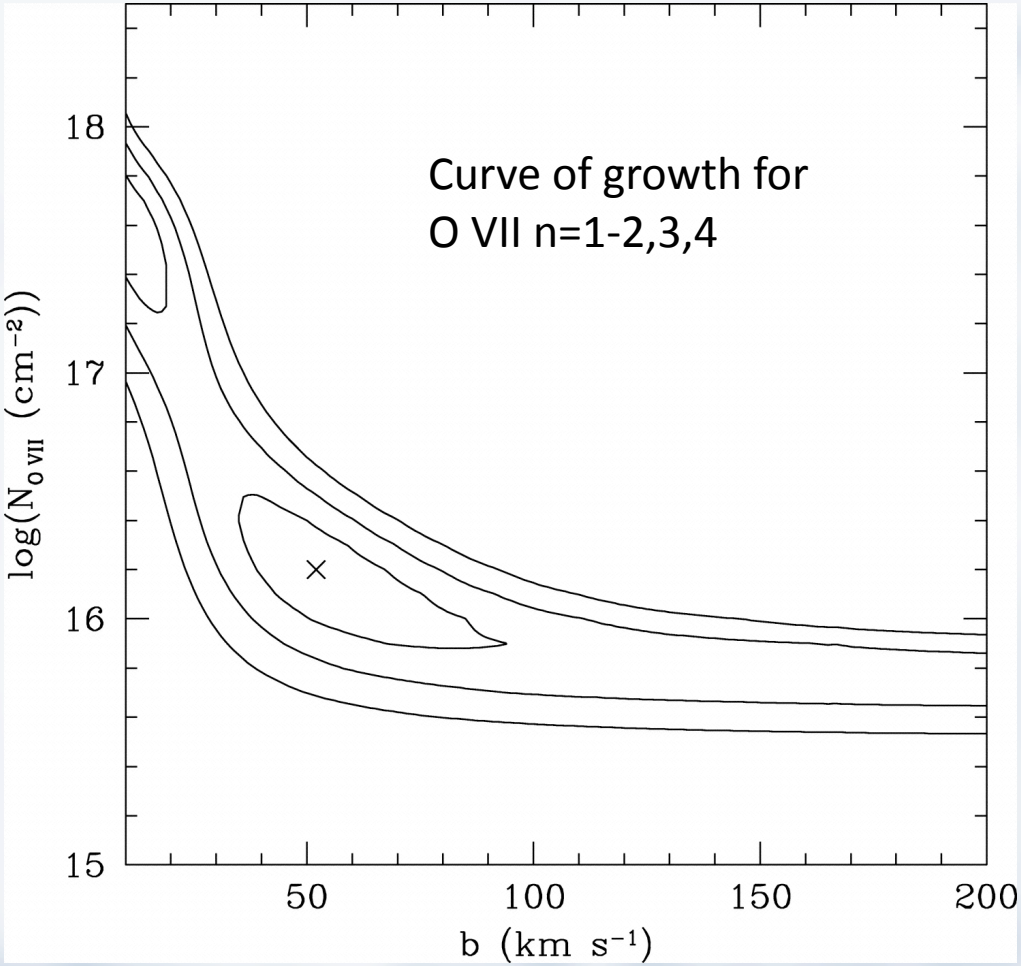
Interstellar/Intergalactic absorption towards blazar PKS2155-304 (z=0)

(Williams et al., *et al.,* 2007, *ApJ,* **665**, 247)



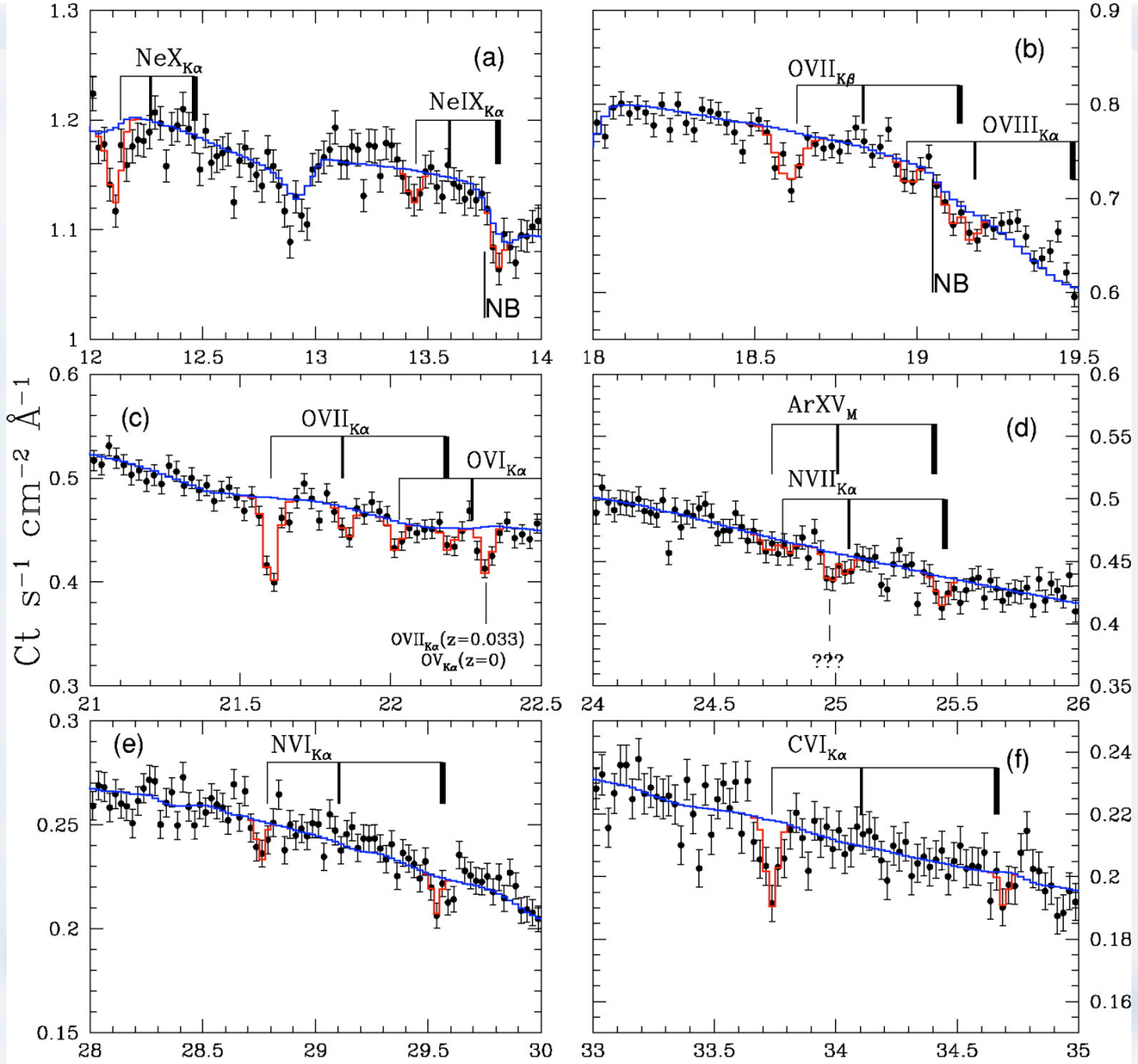
Chandra LETGS, two different focal plane detectors

State of absorbing gas towards PKS2155-304: hot ISM, hot Galactic halo, Hot gas in the Local Group:



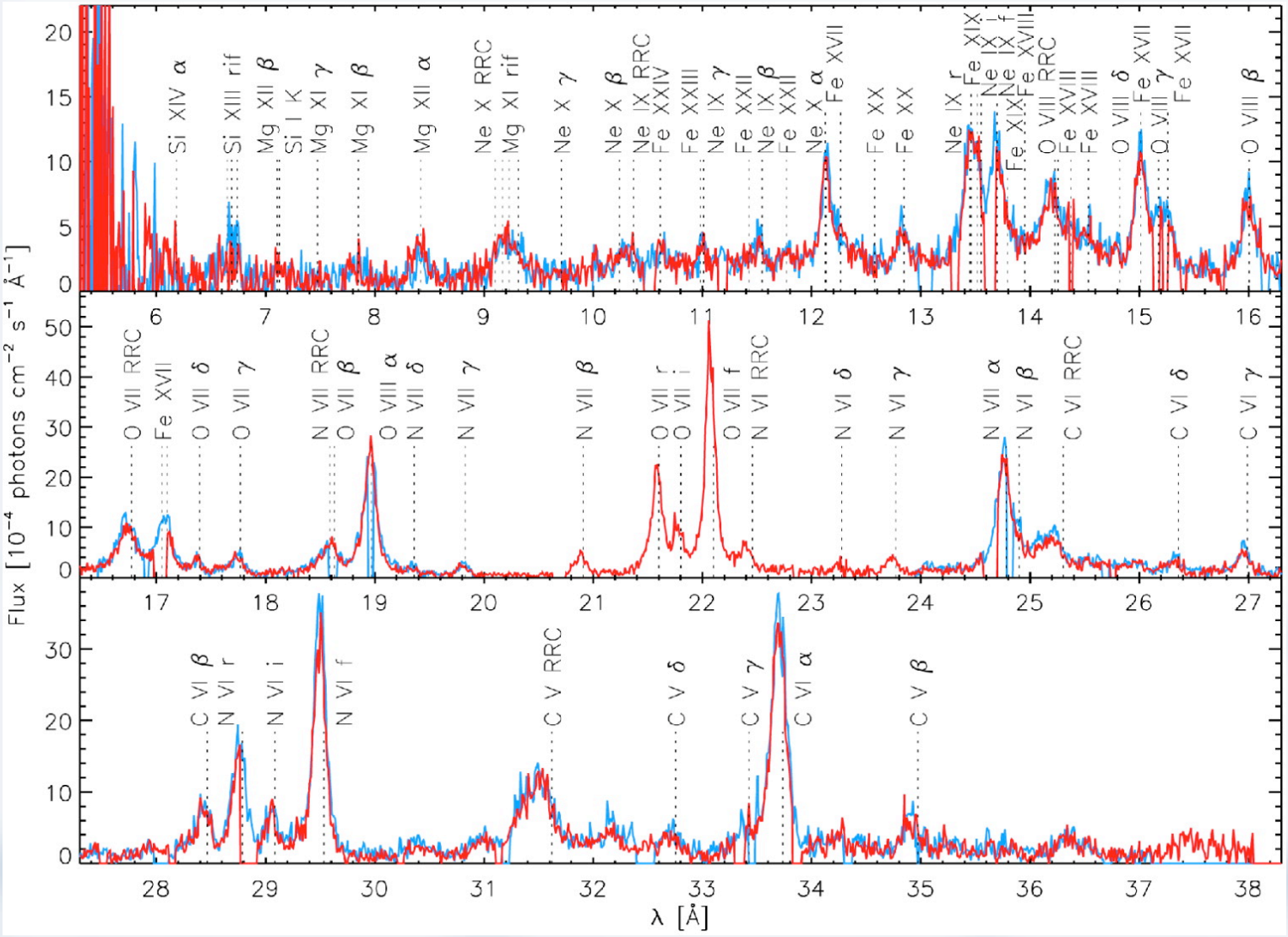
For ***un***saturated lines: EW depends linearly on *N*, independent of *b* (Doppler broadening); Here, n=1-2 evidently saturated. To get EW right for both n=1-2 and n=1-3 requires adjusting both *N* and *b*. In this case, requires gas temperature T ~ 2 x 10^6 K!

IGM absorption, Mkn 421/*Chandra* LETGS

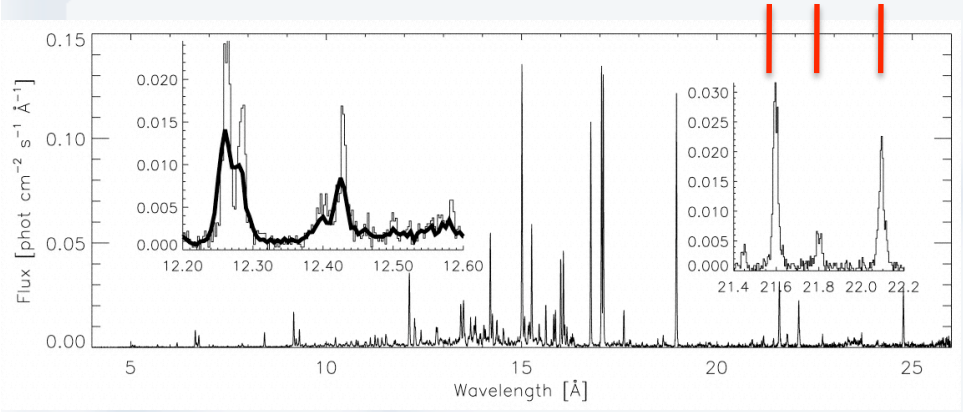


Nicastro et al., 2005, *ApJ*, **629**, 700

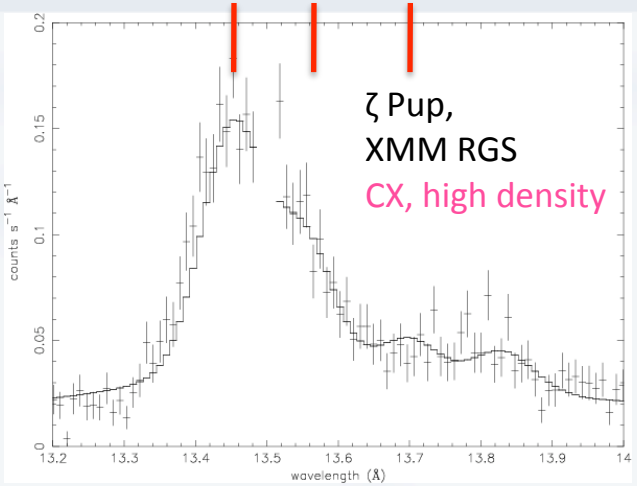
Emission from X-ray photoionized gas



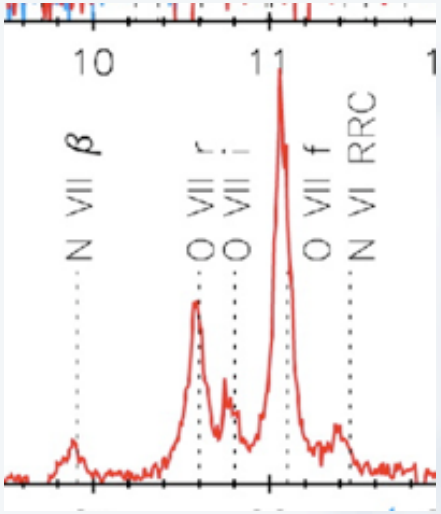
NGC 1068 (Seyfert 2); *XMM-Newton* RGS; Kinkhabwala et al., 2002, *ApJ*, **575**, 732



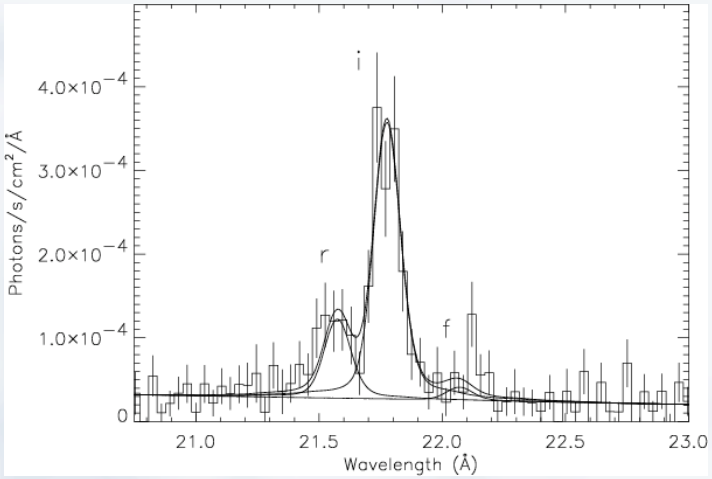
Capella, *Chandra* HETGS:
CX, low density



ζ Pup,
XMM RGS
CX, high density



NGC 1068, RGS
XP, low density



The various faces of the He-like triplets:
Four examples of O VII n=1-2

EXO0748-676, RGS
XP, high density

Resources:

- S. M. Kahn*: Soft X-ray Spectroscopy of Astrophysical Plasmas*, in *High-energy spectroscopic astrophysics* (Saas-Fee Advanced Course 30), Springer, Berlin (2005). Compact and complete primer on atomic physics for X-ray spectroscopy.
- R. W. P. McWhirter: *The contribution of laboratory measurements to the interpretation of astronomical spectra* (Saas-Fee Advanced Course 5), Geneva Observatory (1975). Out of date of course, but very readable, and an excellent 'primer' in X-ray emitting collisional plasmas.
- Jelle Kaastra et al.: *Thermal Radiation Processes*, *Space Sci. Rev.*, **134**, 155 (2008); arXiv:0801.1011. Very nice introduction to the properties of collisional plasmas-ionization balance, spectroscopy, etc.
- Duane Liedahl: *The X-Ray Spectral Properties of Photoionized Plasma and Transient Plasmas*, in *X-ray Spectroscopy in Astrophysics*, Lecture Notes in Physics, **520**, p.189 (Springer, 1999). A pedagogically excellent introduction to photoionized and non-equilibrium plasmas. **Accessible through ADS.**
- reviews of recent results:
  Paerels and Kahn, *Ann. Rev. Astron. Astrophys.*, **41**, 291 (2003)
  Claude Canizares et al., *Publ. Astron. Soc. Pac.*, **117**, 1144 (2005)