Absorption Spectroscopy

Frits Paerels (*)/Columbia University
AtomDB Workshop, Tokyo Metropolitan University
September 2014

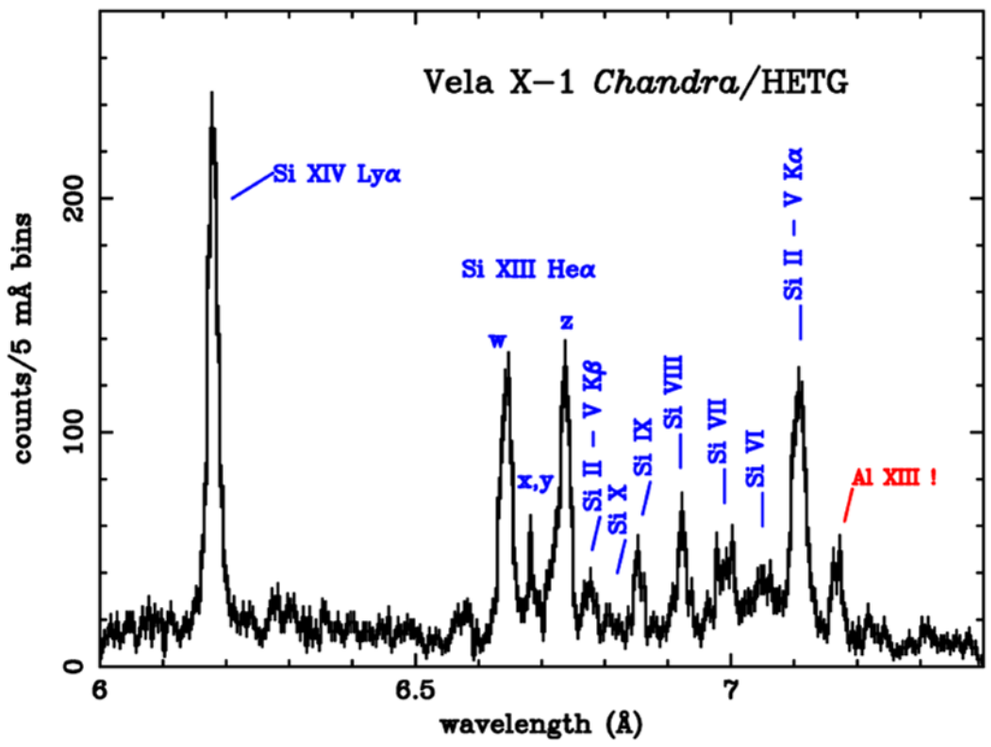
(*) standing on the shoulders of many others

Absorption Lines

X-ray band (~0.1-10 keV) contains spectra of all ionization stages of all abundant elements

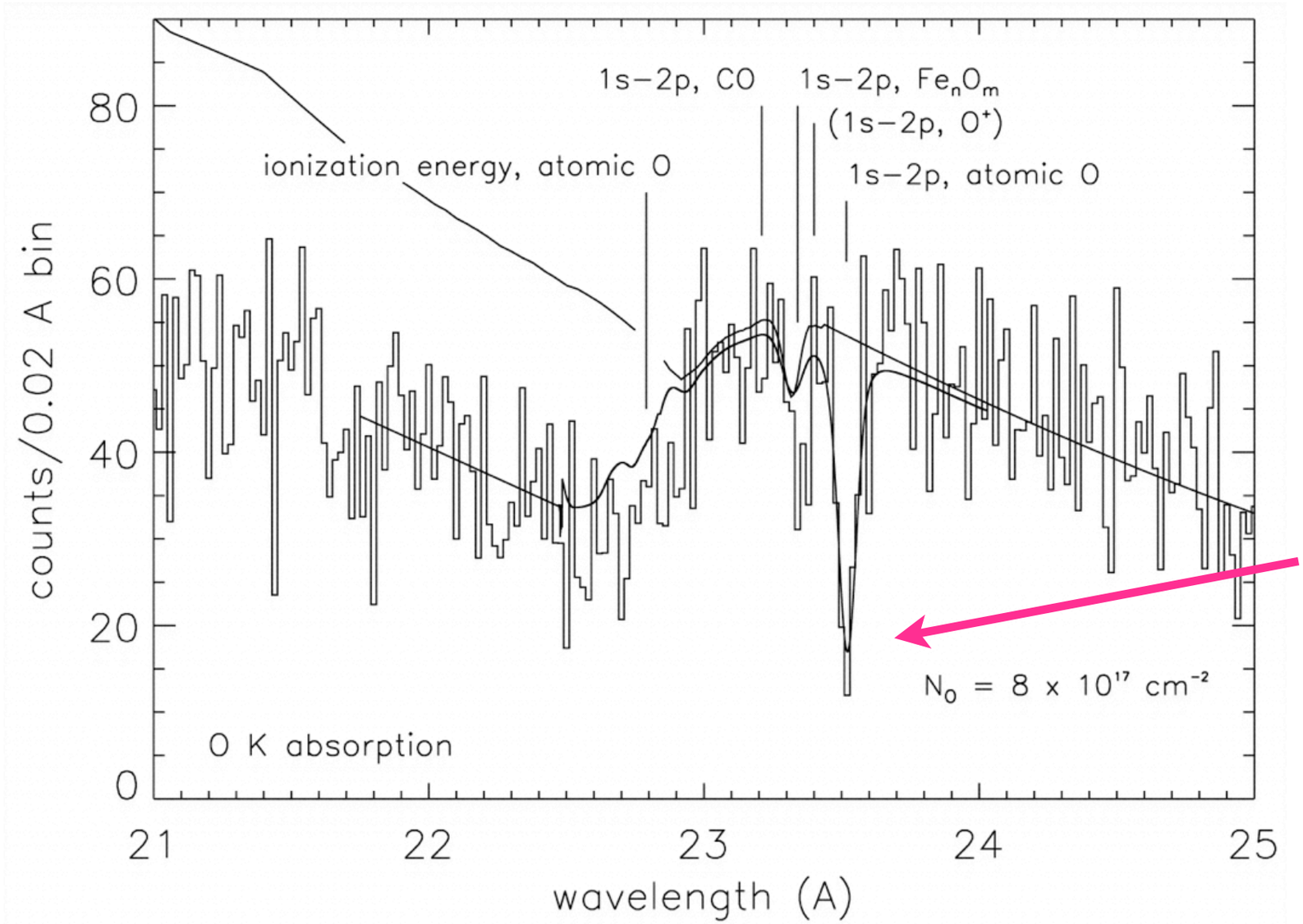
($E_0 \sim Z^2$.Ry, Z = 6, 7, 8, 10, ..., 26)

Wide range of ionization usually in *absorption* spectra; emission usually from limited range of ionization



example actually from emission...
emission from the stellar wind in Vela X-1:
all ionization stages of Si in one spectrum!

Anything that changes the structure of the valence shell (ionization; chemical binding) shifts its energy by ΔE ~ eV per electron: position of absorption lines changes by ~ 1 part in few 100 - 1000



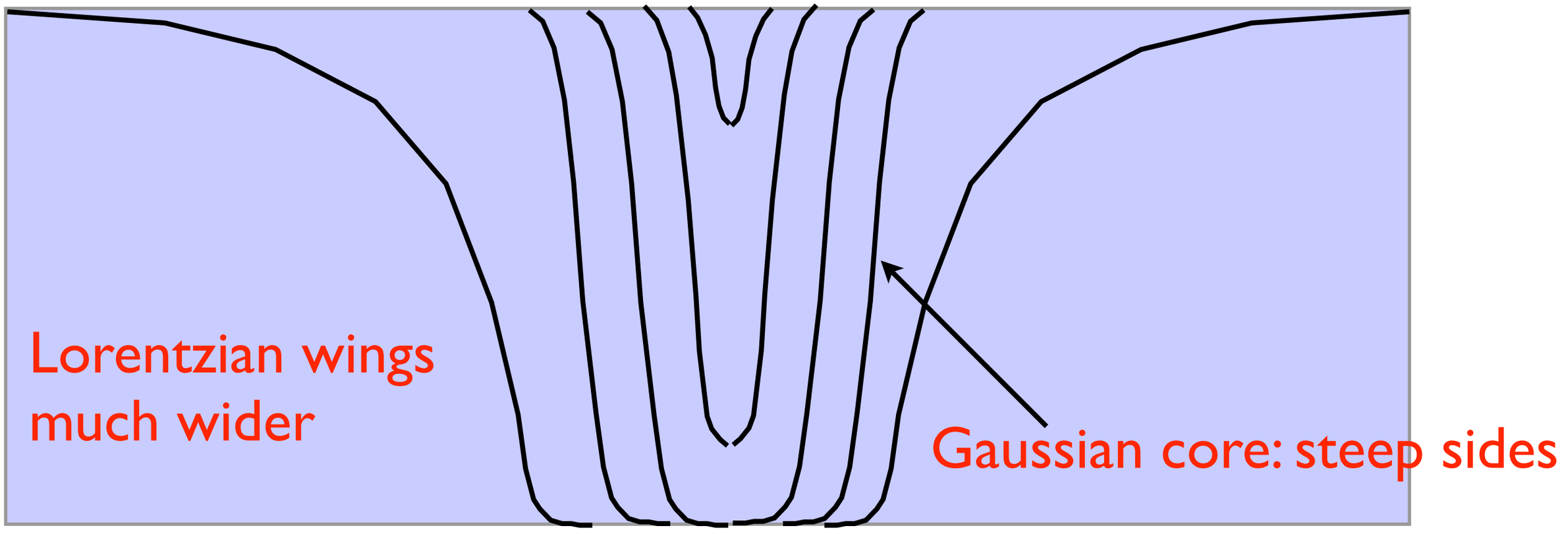
X0614+091
Chandra LETGS
FP *et al.* 2001

saturated!
(N_O derived from edge depth)

absorption lines more sensitive than continuum edges
to small absorber column densities

convert absorption line ‘strength’ into column density:
straightforward, but be careful with saturation

absorption line saturation



absorption line ‘strength’: *equivalent width (EW)*
(area of equivalent rectangle under continuum)
(NB: independent of spectrometer resolution!!!)

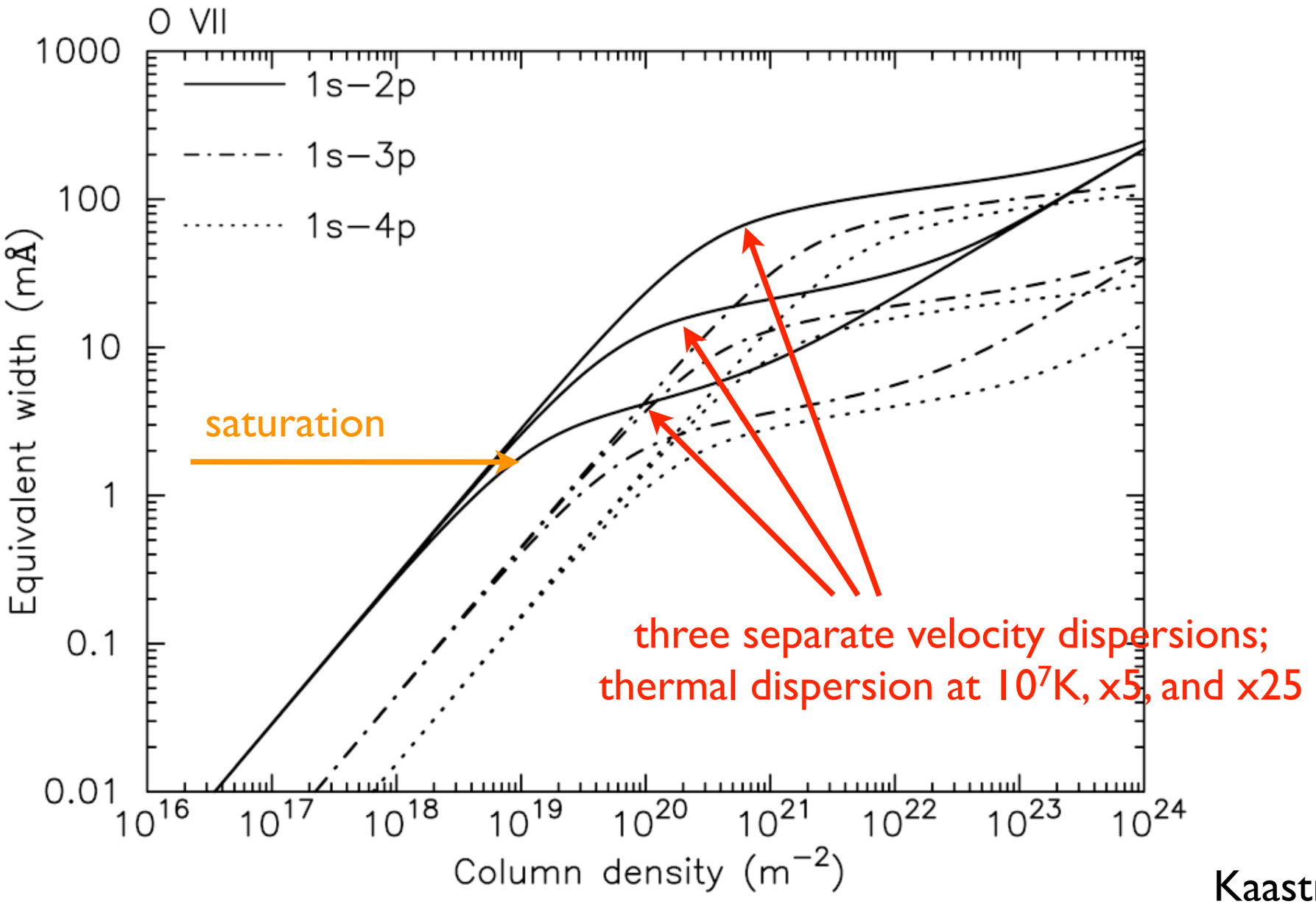
Saturation EW ~ line core width;
often (??) thermal velocity dispersion:

$$\frac{v}{c} \sim \left(\frac{kT}{M_i c^2}\right)^{1/2} = \frac{1}{13000}\left(\frac{M_i}{16 m_p}\right)^{-1/2}\left(\frac{T}{10^6\ \mathrm{K}}\right)^{1/2}$$

moderate saturation basically not diagnosable in
unresolved lines
circumvent: see higher order series members: do ‘COG’

the 'Curve of Growth'

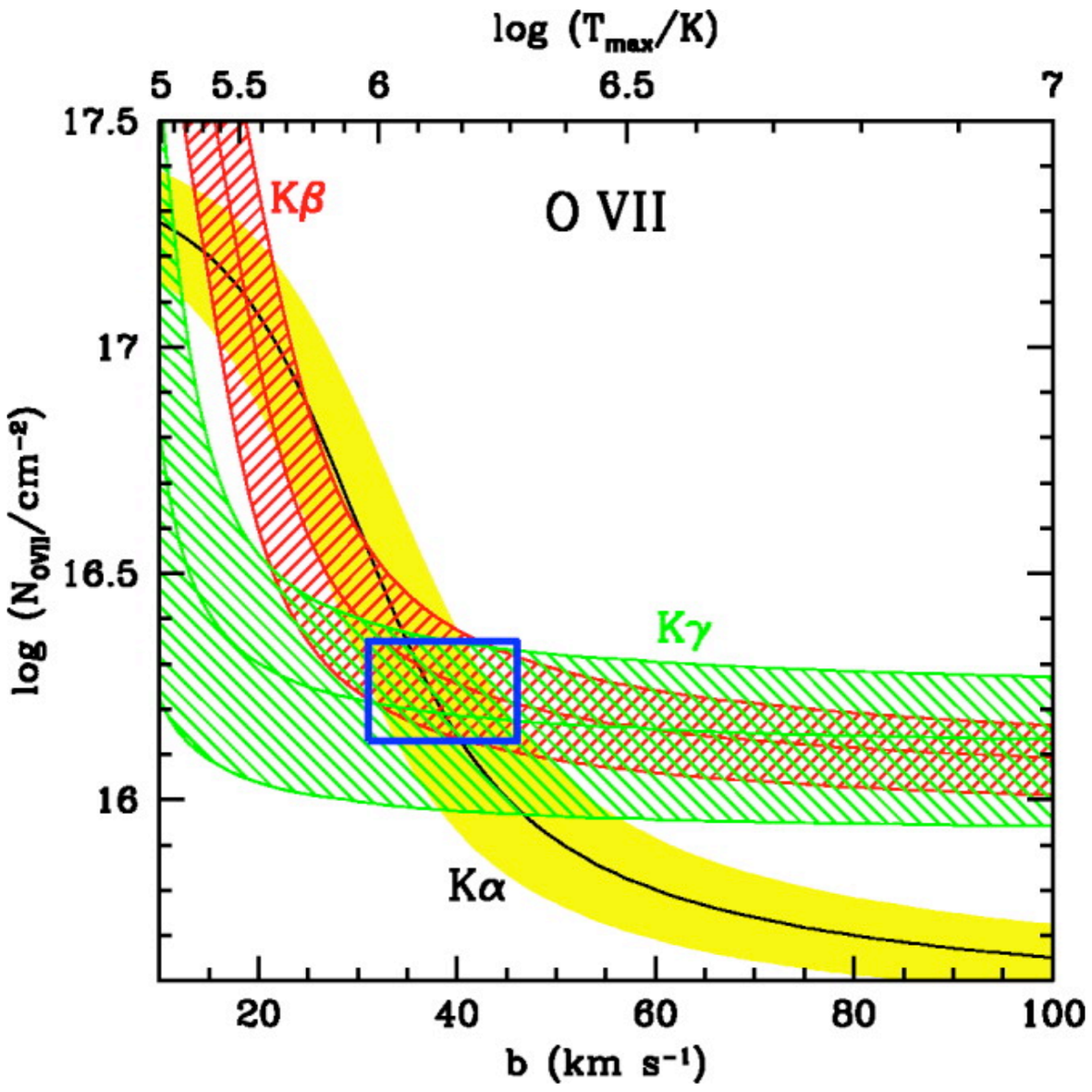
'curve of growth': EW vs. absorber column density

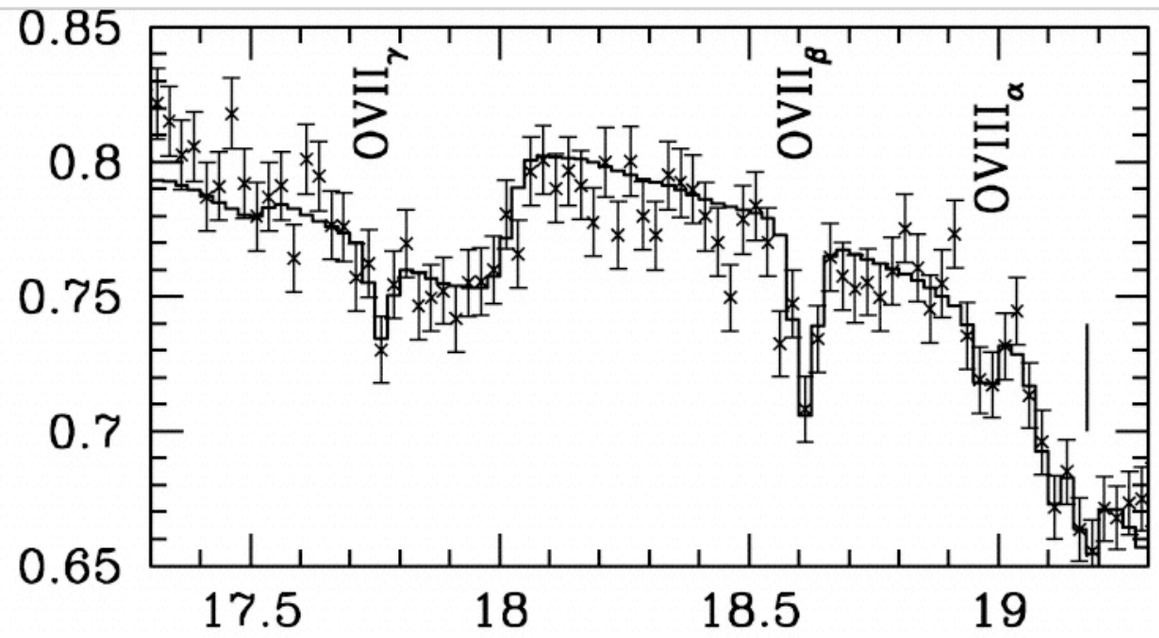


Kaastra *et al.* 2008

NB: resolving 1 mA in O VII resonance line requires R ~ 20,000!!!

higher order series members:
cross section typically order of magnitude smaller than n=1-2:
saturate at much higher column density





circumgalactic absorption, Mkn 421 *Chandra* LETGS; Williams *et al.* 2005

Photoelectric Absorption Edges

1. Far above the ionization energy
2. Close to the ionization energy; XANES, (E)XAFS, ...

1. Far above the ionization energy (but not relativistic)

perturbation theory:

cross section $\propto \left| \langle \psi_{\mathrm{final}} \left| H_{\mathrm{int}} \right| \psi_{\mathrm{initial}} \rangle \right|^2$

free photoelectron in Coulomb field of ion

incident radiation field

bound atomic state

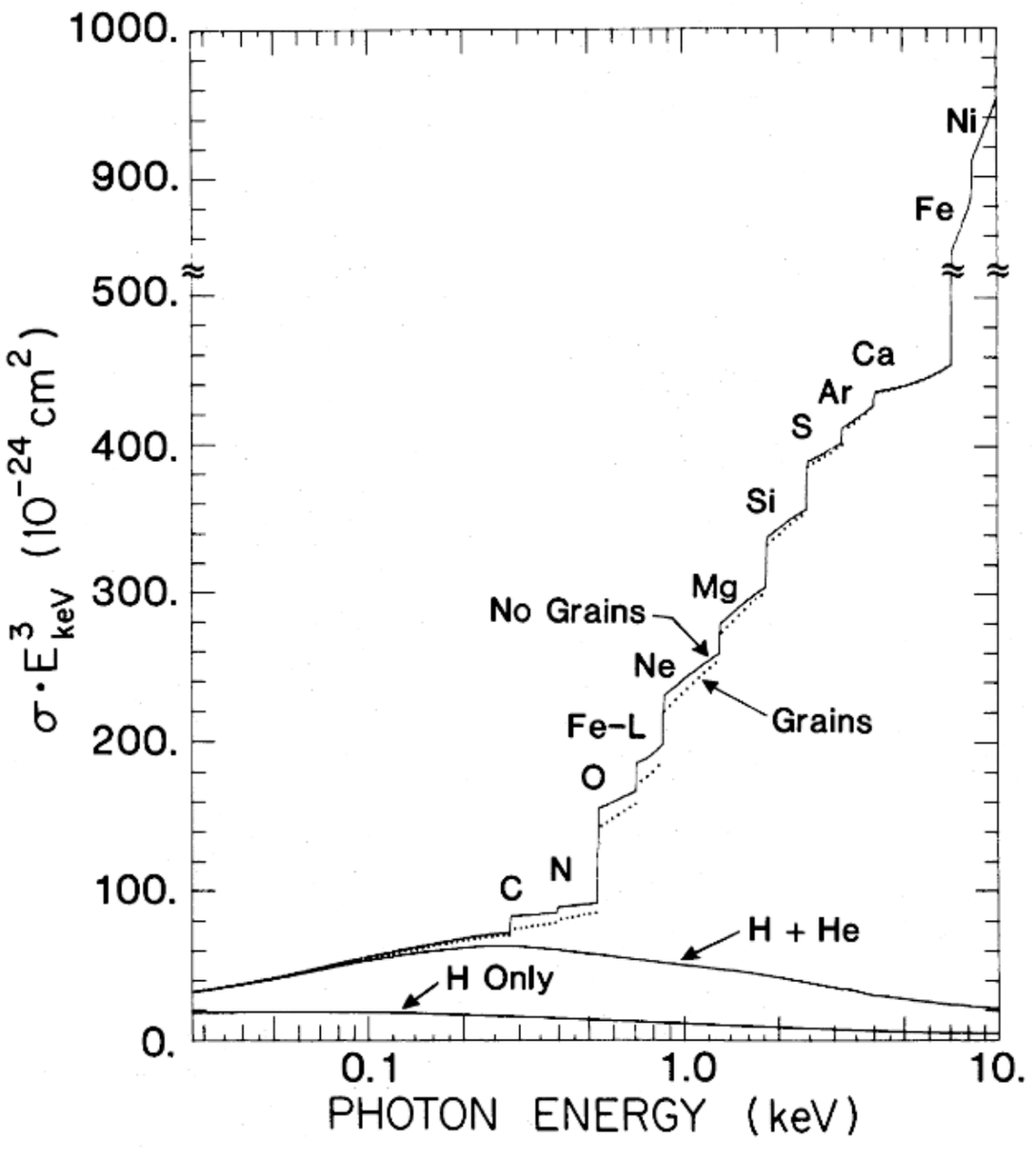
free electron ~ plane wave;
dipole approximation for radiation field: exp(*i**k**.**r*) → 1

$$\sigma = 4\sqrt{2}\ \sigma_{\mathrm{T}}\alpha^4 Z^5 \left(\frac{m_e c^2}{\hbar\omega}\right)^{7/2}$$

Thomson cross section

at K threshold: $E_K = Z^2.Ry$, so
$\sigma \sim$ constant Z^{-2}

cross section of the ISM;
Morrison & McCammon 1983



1a. Intermezzo: autoionizing resonances in continuum cross sections

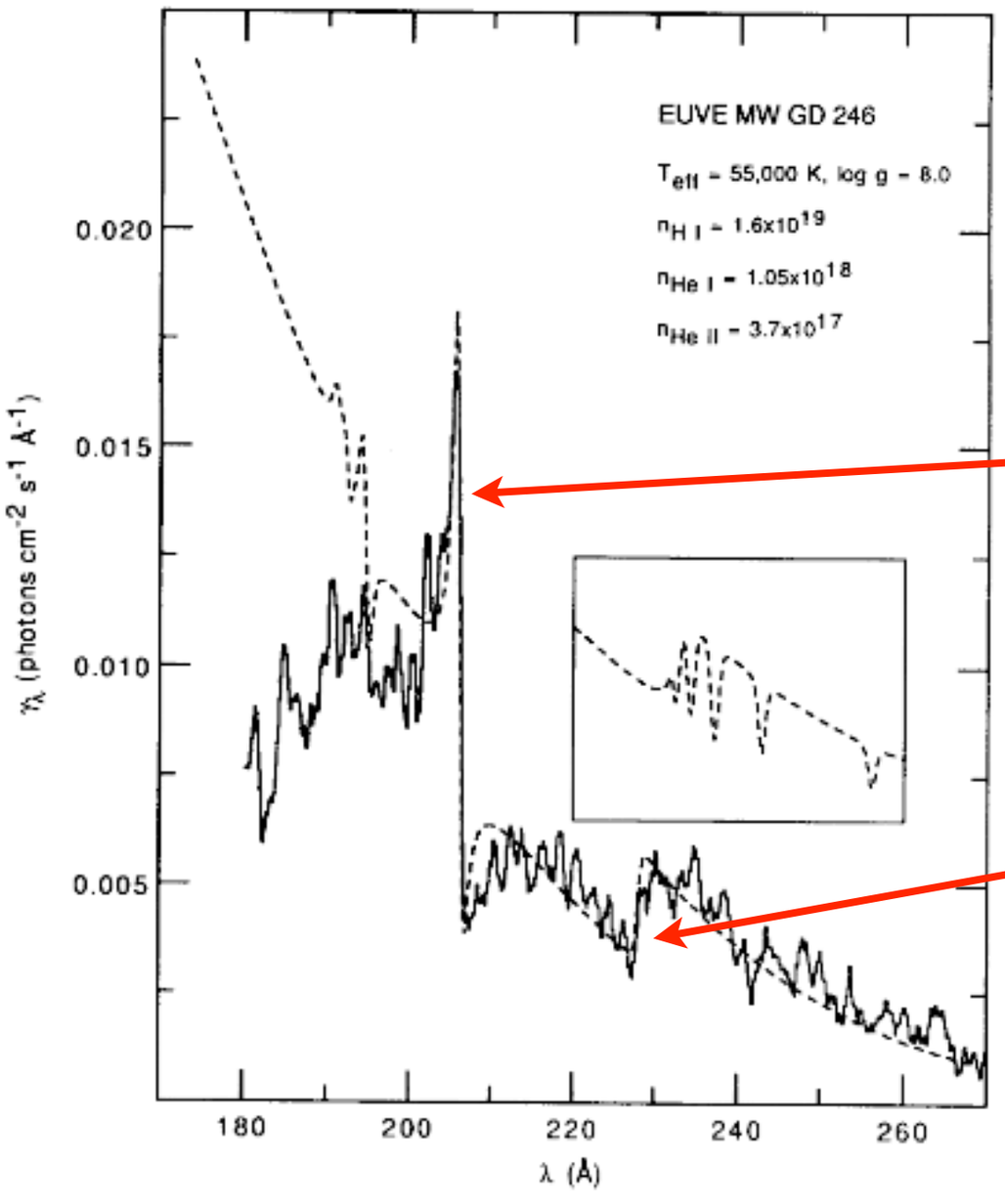


FIG. 1.—Pure H synthetic spectrum adjusted to the observed EUV spectrum of GD 246 in the range $\lambda \geq 200$ Å (see § 3.1). *Inset:* Synthetic spectrum with a trace abundance of helium (He/H = 2×10^{-5}) illustrating pressure broadening effects near the He II series limit in a model atmosphere.

interstellar absorption in hot DA white dwarf GD246

He I autoionization resonance (ISM)

He II Ly edge (ISM)

Vennes *et al.* 1993

autoionizing resonances in continuum cross sections

$$h\nu + \mathrm{He} \rightarrow \mathrm{He}^{**} \rightarrow e^- + \mathrm{He}^+$$

$2\ell n\ell'$; e.g. $2s2p$; $E <$ ionization energy

autoionization; $h\nu$ destroyed

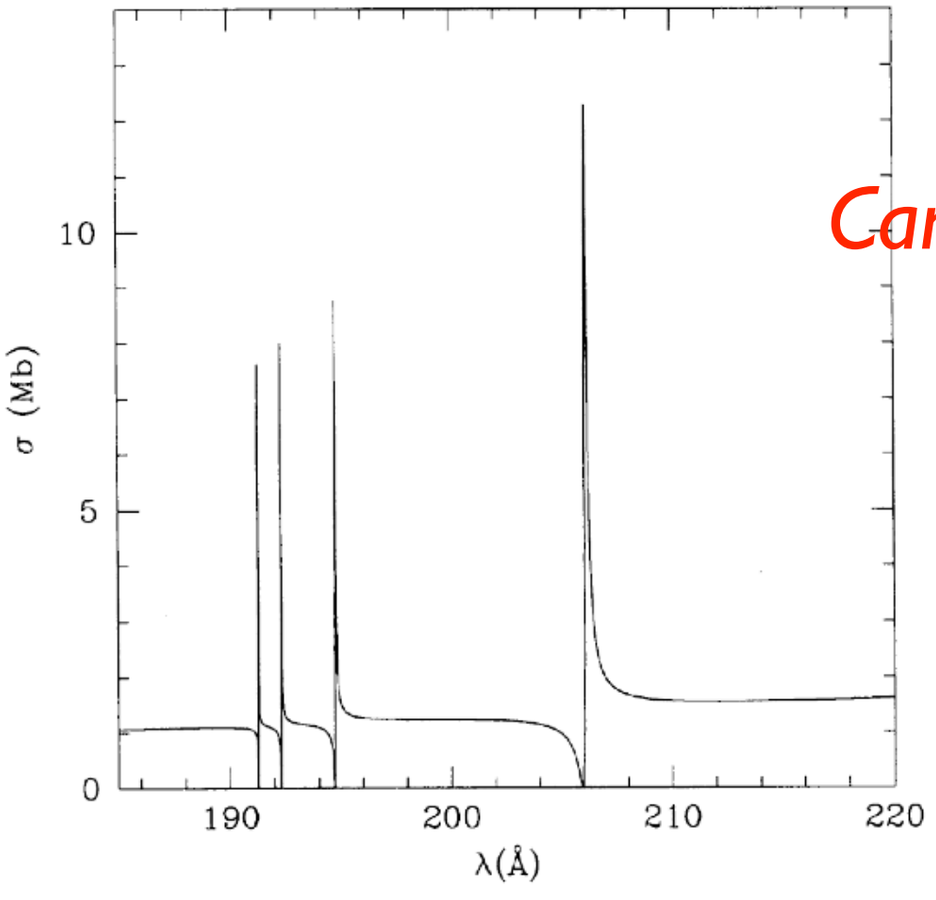


FIG. 1. The photoionization cross section of He I showing the first four $(sp, 2n+)^1P^0$ autoionizing resonances. Cross sections are given in Mb (10^{-18} cm).

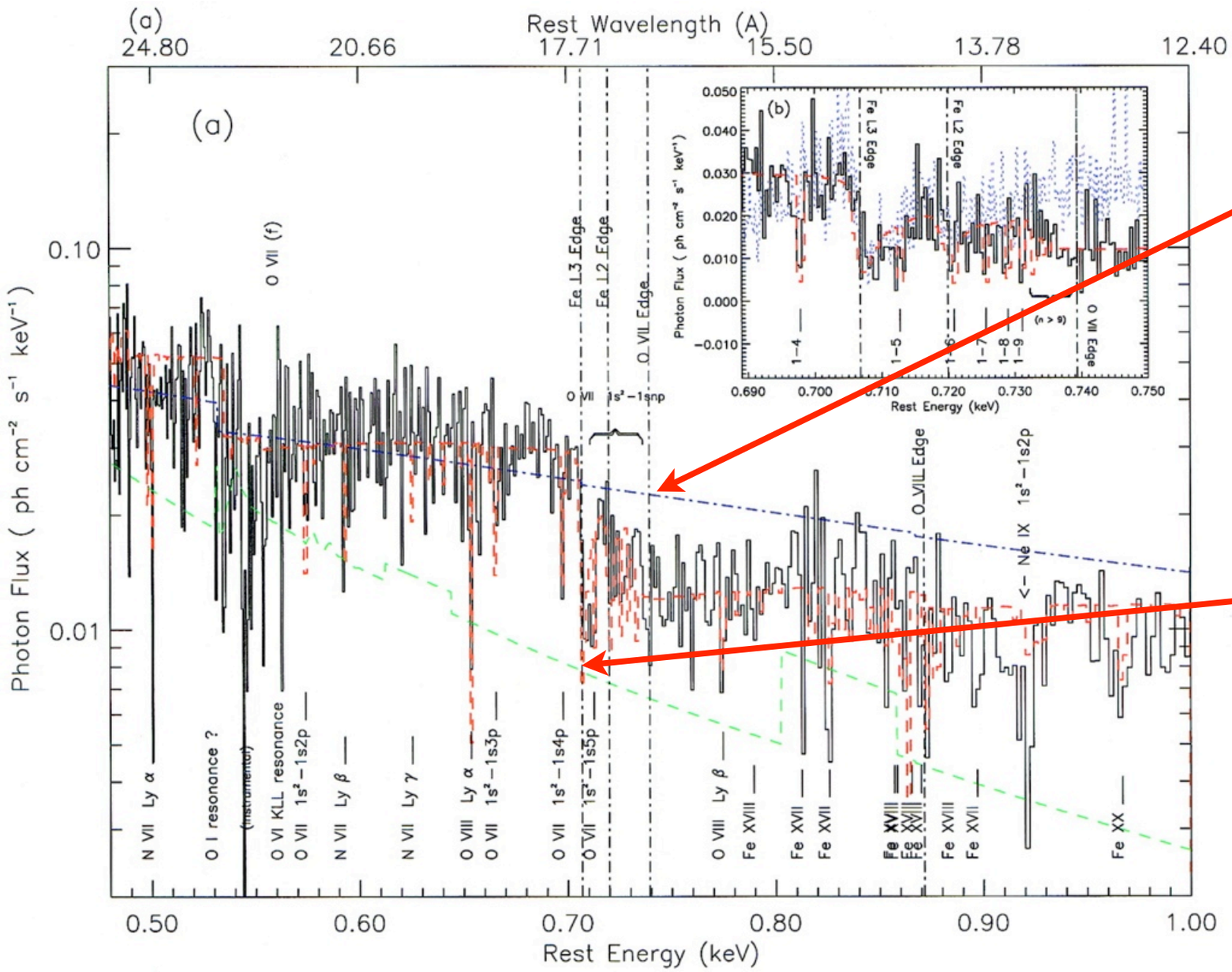
Can we see this in C V, O VII, Ne IX, ...?

He I; Rumph *et al.* 1994

2a. Close to the ionization energy (atomic absorption)

Few-electron ions: example O VII

O VII series limit 'eroded' by presence of multiple, weak, unresolved lines converging on limit



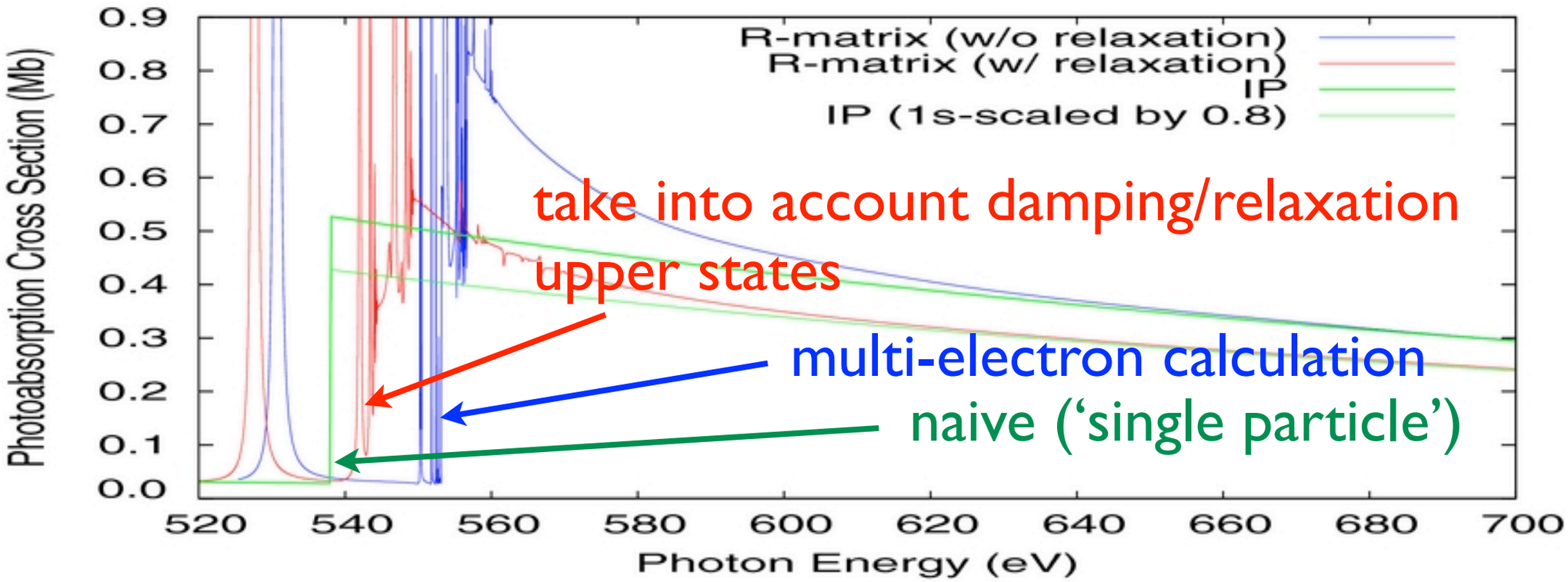
Also note presence of Fe L $2p_{1/2}$,$2p_{3/2}$ "edges" (see later)

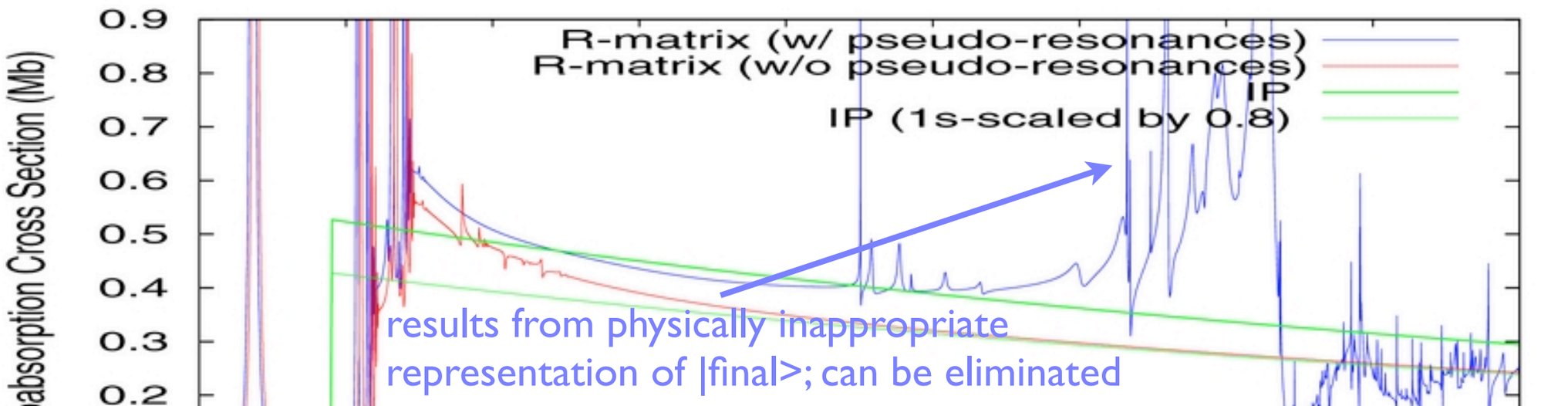
MCG-6-30-15, *Chandra* HETGS/Lee *et al.* 2001

2a. Close to the ionization energy (atomic absorption)

many-electron ions/atoms

O I K absorption; R-matrix, Gorczyca *et al.* 2013;
note importance of detailed treatment of all possible decays from upper state!
(blue → red)

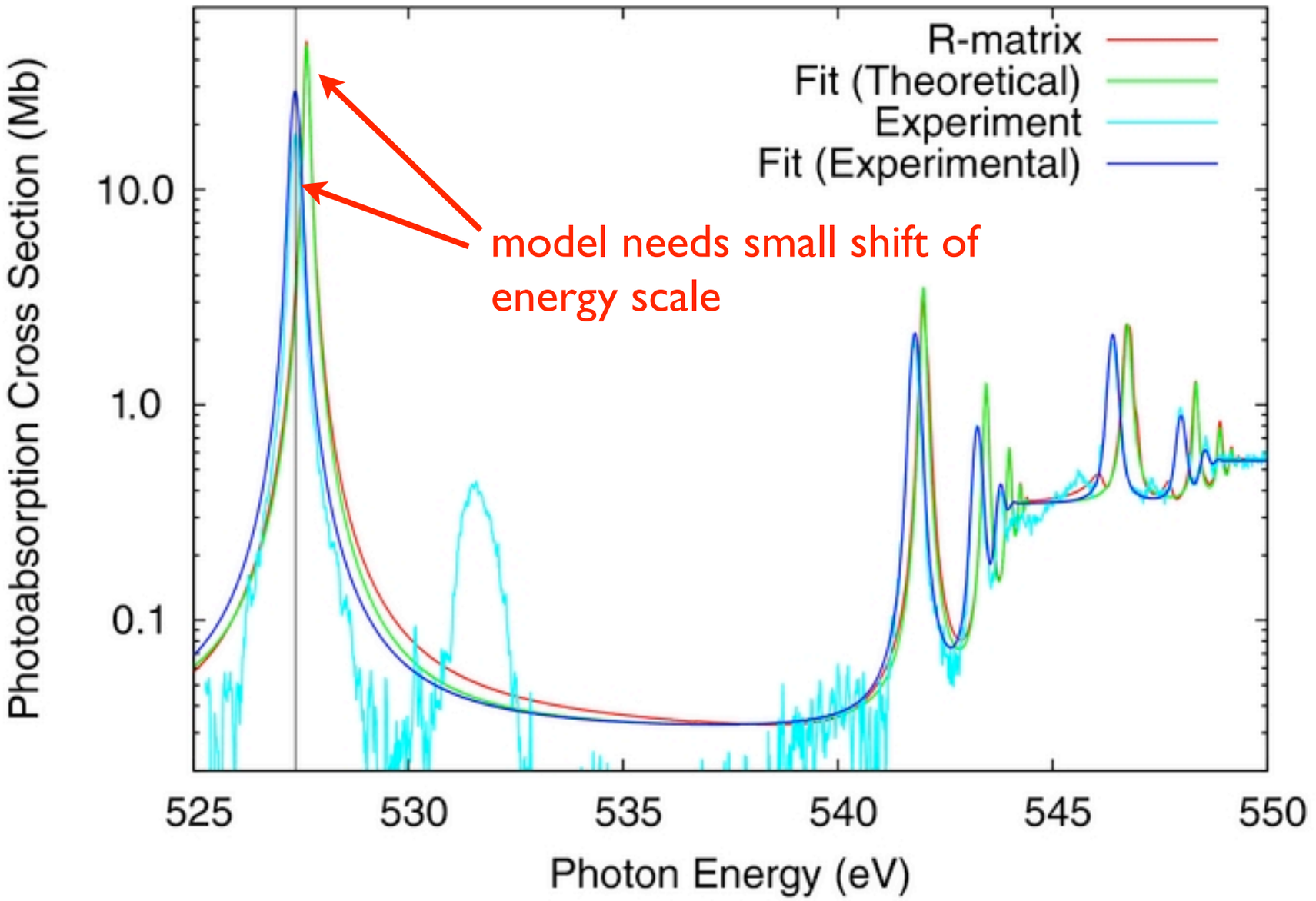




2a. Close to the ionization energy (atomic absorption)

many-electron ions/atoms

zoom in; compare to experiments
(difficult to make monatomic O!!)



model convolved with
0.18 eV FWHM Gauss
to match experimental
resolution

2a. Close to the ionization energy: atomic absorption

many-electron ions/atoms

how well does this stuff do?

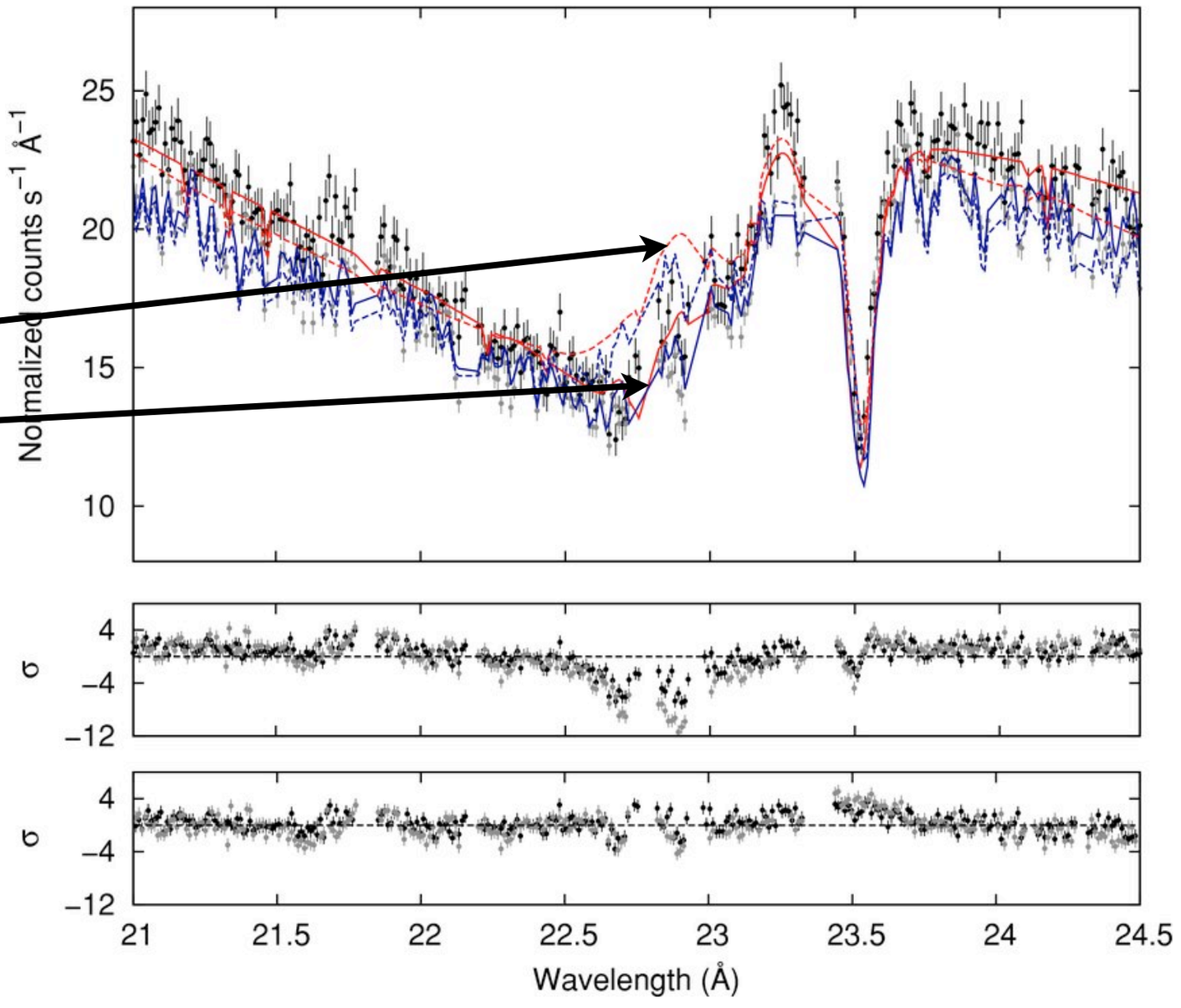
Sco X-1 XMM/RGS

---- 'old' calculation

—— 'new' calculation

residuals 'old'

residuals 'new'



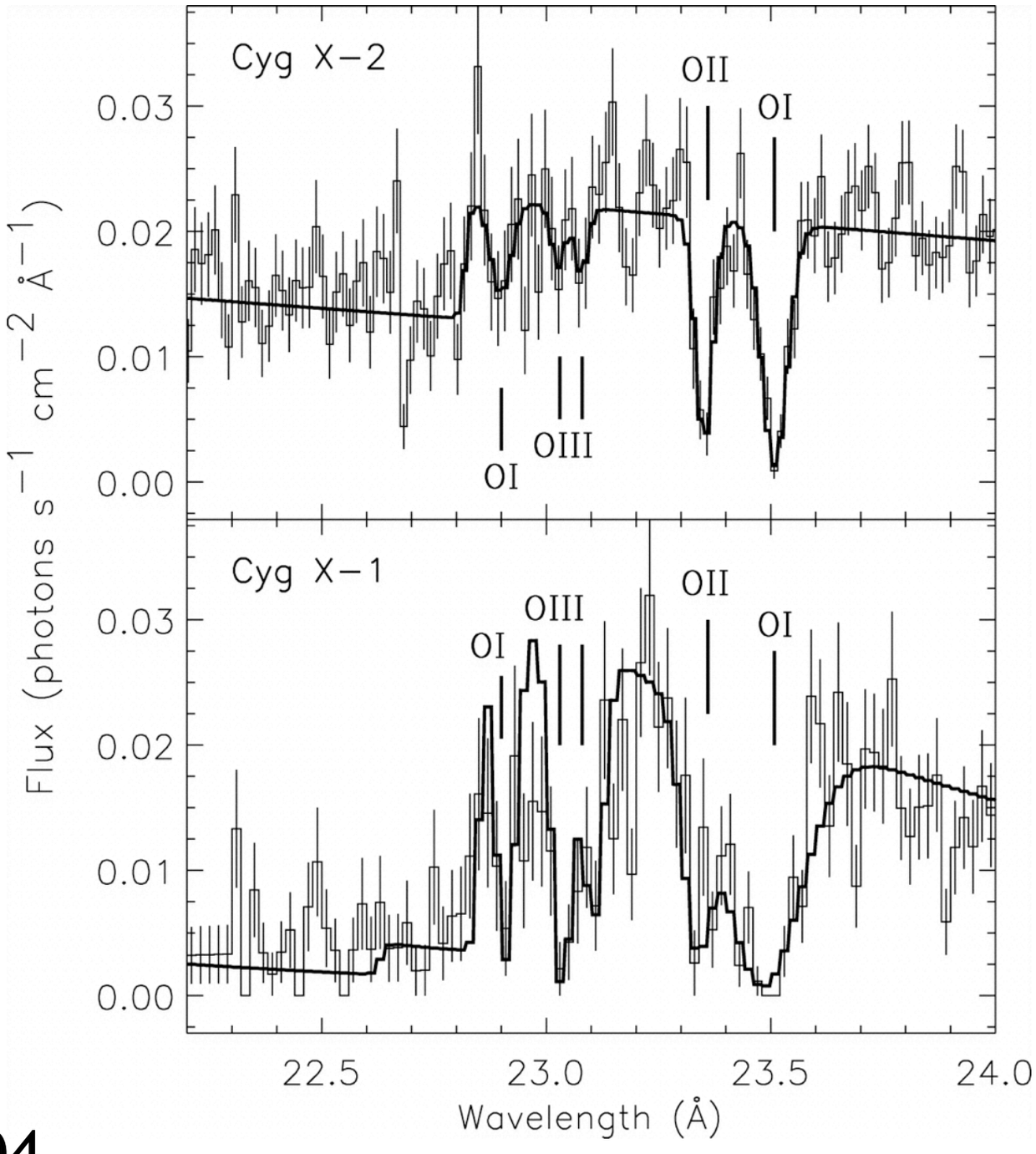
blue/red:
two different datasets

Garcia *et al.* 2011

2a. Close to the ionization energy: atomic absorption

many-electron ions/atoms

effect of ionization



Chandra HETGS/ Juett *et al.* 2004

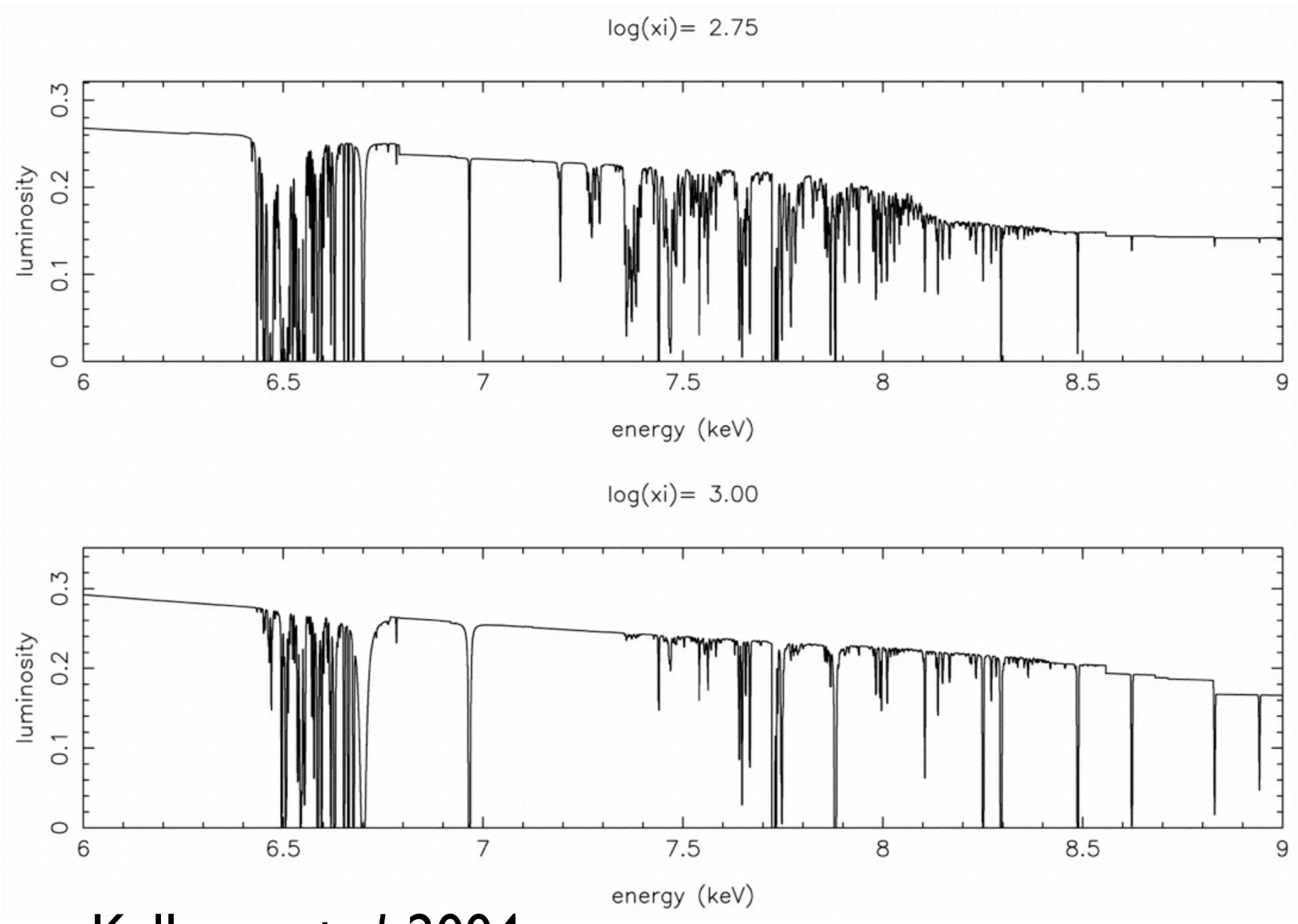
2a. Close to the ionization energy: atomic absorption

many-electron ions/atoms

innershell absorption by Fe

gas in photo-ionization equilibrium; fixed ionization parameter

this example: mostly L-shell ions contributing



Kallman *et al*. 2004

2b. Close to the ionization energy: absorption in molecular and solid phase XANES, (E)XAFS, ...

definition of 'close':
photoelectron momentum:

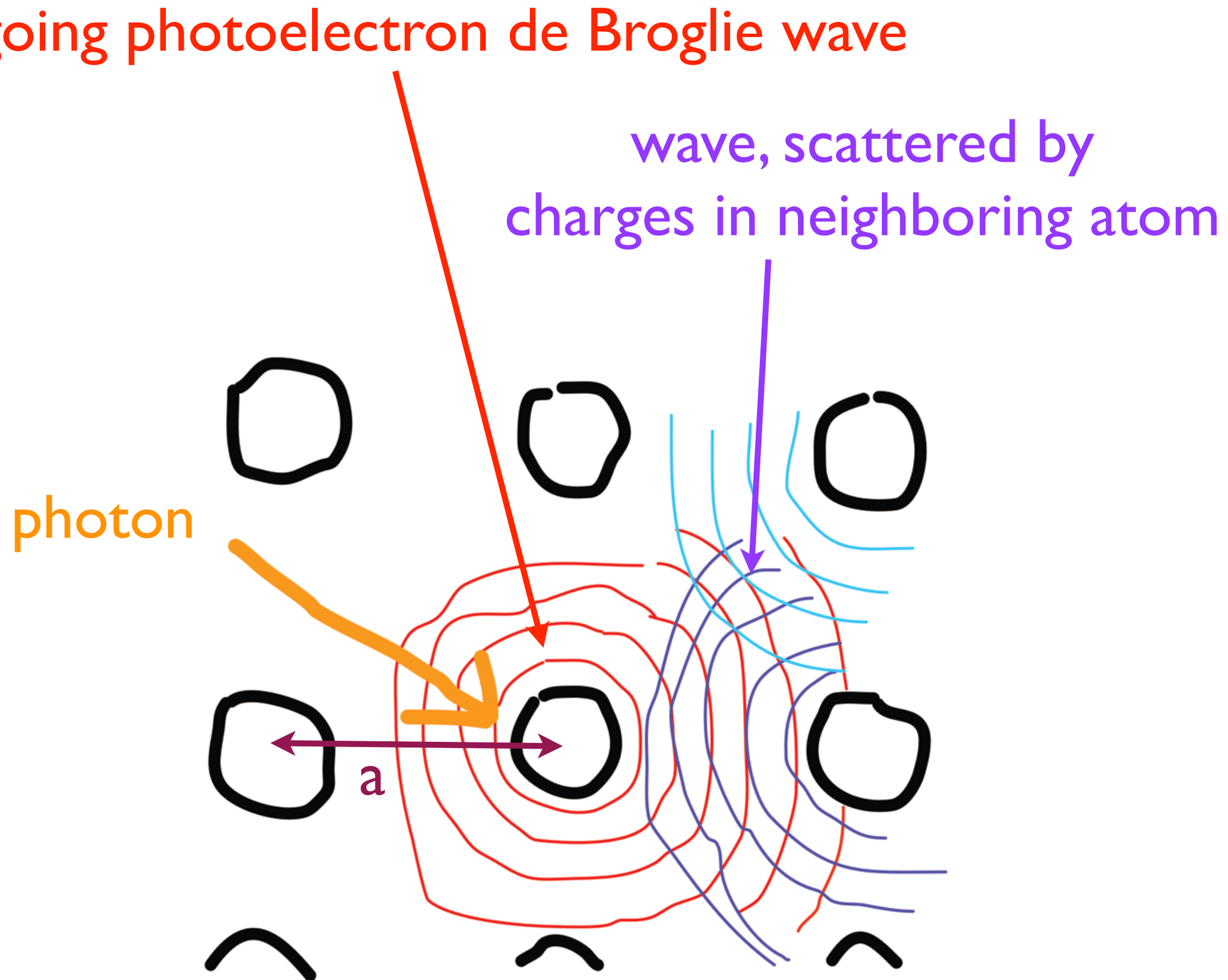
photoelectron de Broglie-wavelength

interatomic distance

$$\frac{\hbar^2 k^2}{2m_e} = E_\gamma - \chi;\ \lambda_e \sim a \ \Rightarrow$$

$$\Rightarrow \quad E_\gamma - \chi \sim \frac{h^2}{2m_e a^2} = 150(a/1\ \text{Å})^{-2}\ \text{eV}$$

why does interatomic distance matter?



why does interatomic distance matter?

transition probability ∝

$$\propto \left|\langle \psi_{\text{final}} \left| H_{\text{int}} \right| \psi_{\text{initial}} \rangle\right|^2 = \left|\langle \psi_{\text{out}} + \psi_{\text{scattered}} \left| H_{\text{int}} \right| \psi_{\text{initial}} \rangle\right|^2$$

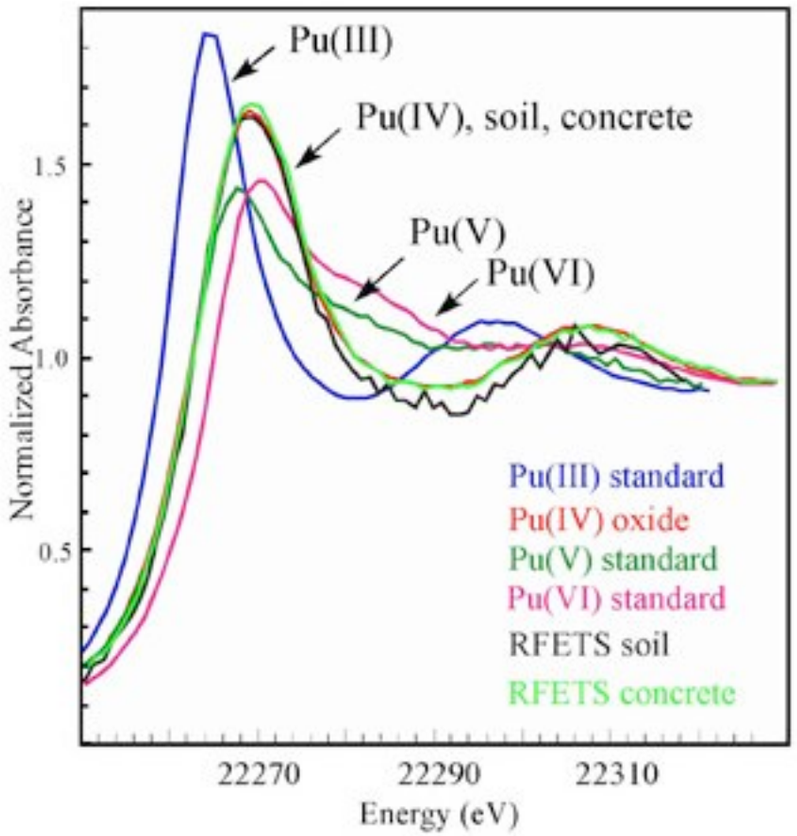
interference! modulates the entire matrix element;
when amplitude of ψ_{out} + $\psi_{scattered}$ is small near absorbing atom (where $\psi_{initial}$ is nonzero):
transition probability suppressed

'resonance': $n\lambda_e \sim a$

note: this does *not* require a full lattice! only short-range order!

Also: $\psi_{scattered}$ is sensitive to nature of scatterer!

from Wikipedia



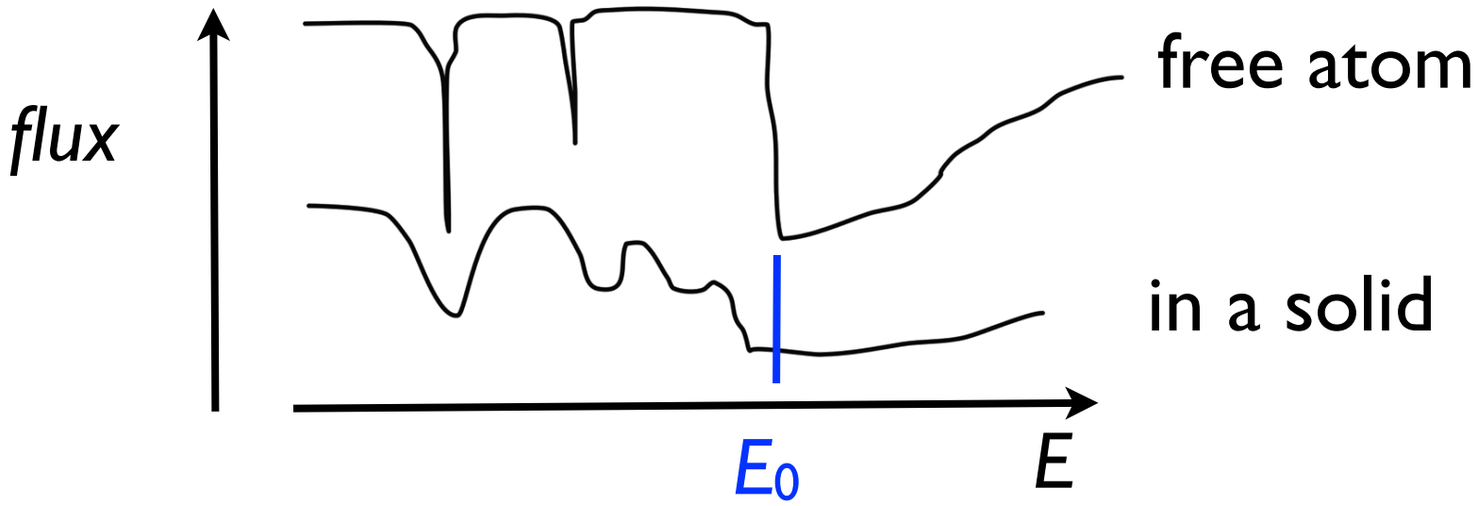
absorption spectrum of Pu
from samples taken near Rocky Flats

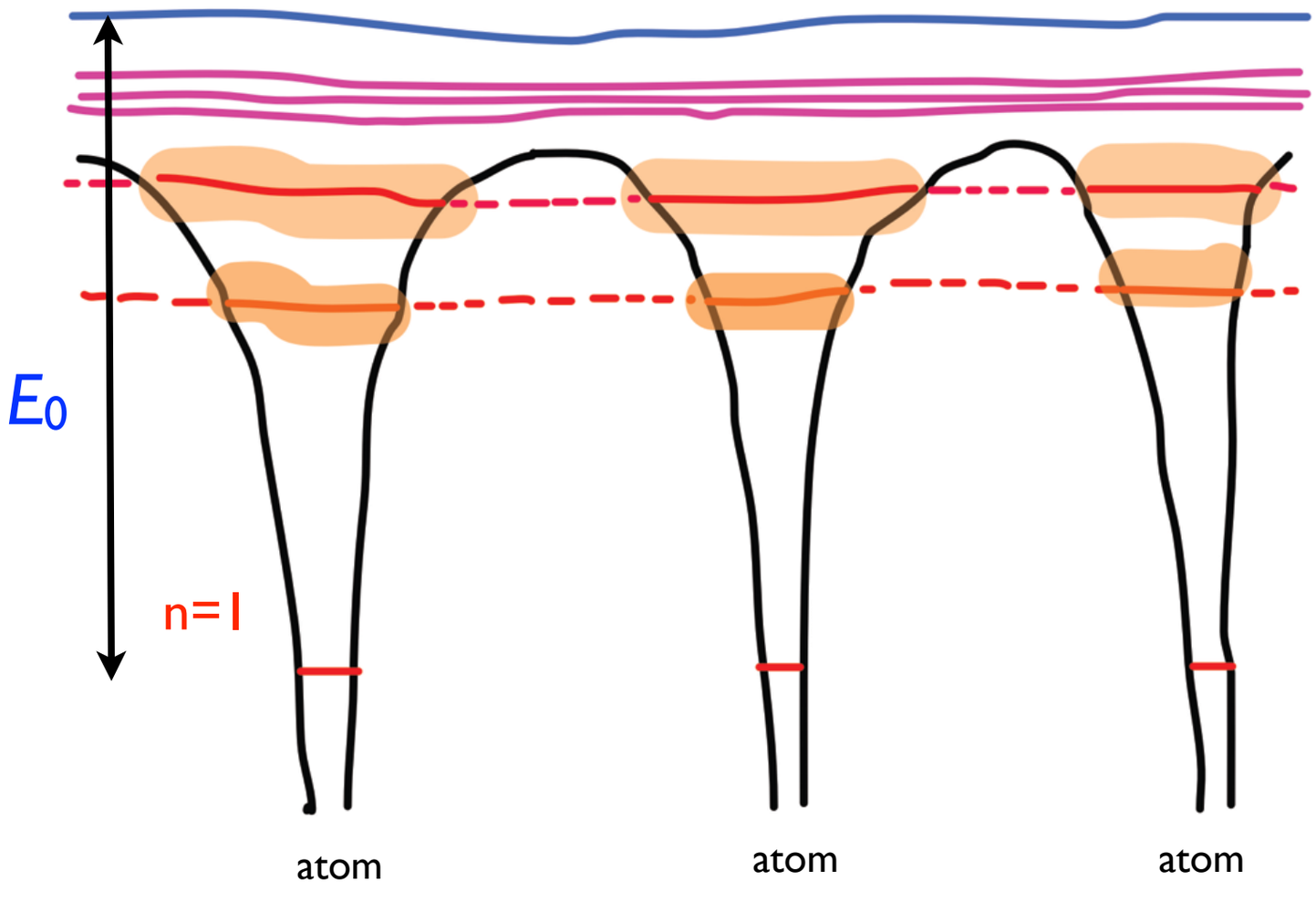
the effect occurs not just in solids, but in any medium with short-range order
(such as molecules in gas phase!)

terminology:
XANES: X-ray absorption Near-Edge Structure
(E)XAFS: (Extended) X-ray Absorption Fine Structure

if $\lambda_e \gtrsim a$: XANES; if $\lambda_e < a$: XAFS

another contributor to XANES: 'band structure'





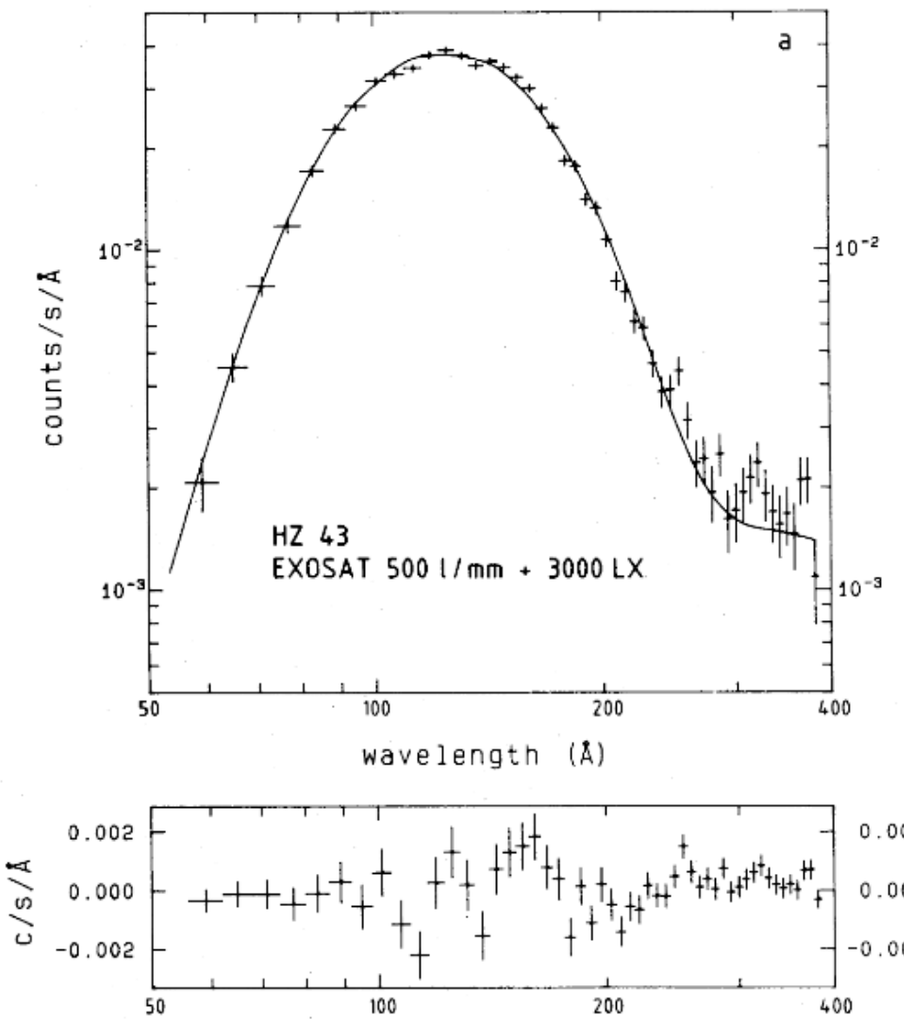
binding energy above n=1 in *free* atoms

free electrons in periodic potential

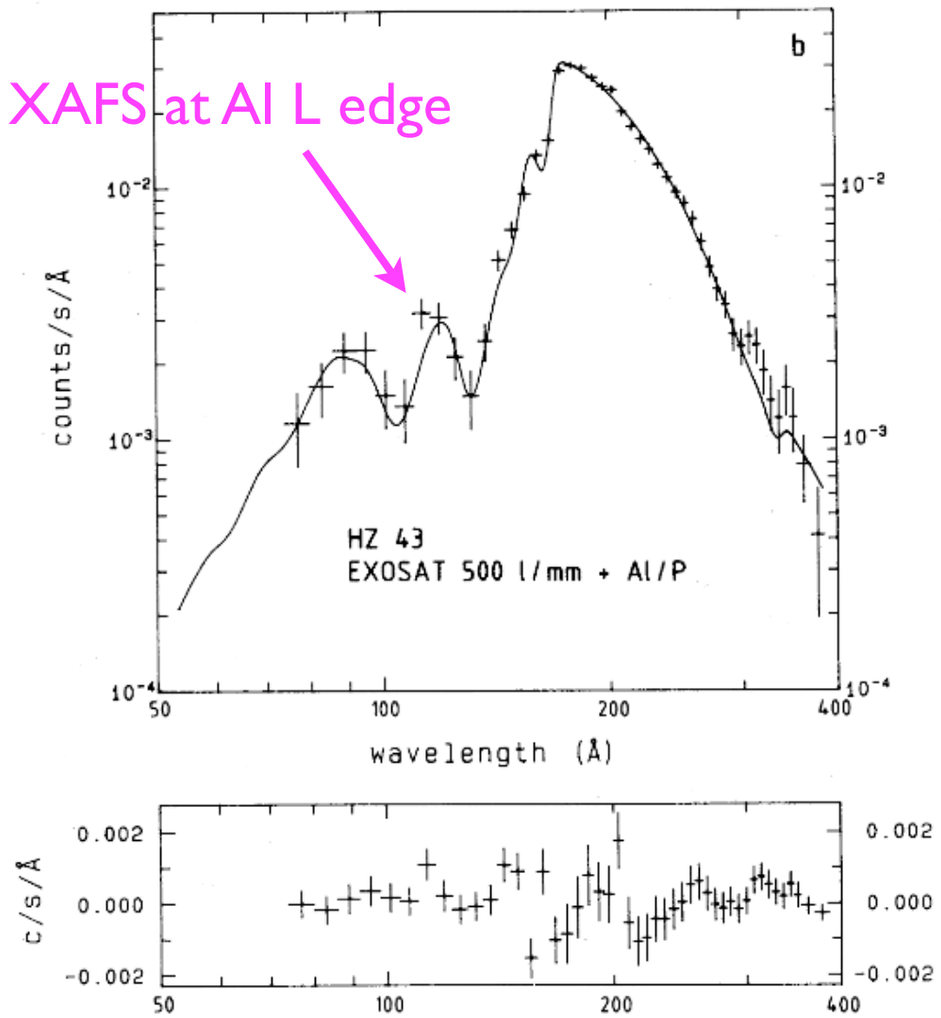
bound levels broadened by tunneling

obvious importance to astrophysics:
(1) instrumental calibration...
(2) molecular and dust absorption in ISM

plastic beam filter



Al beam filter



(very old) example of an instrument calibration issue
hot DA white dwarf HZ43, EXOSAT TGS

FP *et al.* 1986

Interstellar Absorption by molecules and dust

Fe L absorption: the L 'edges'

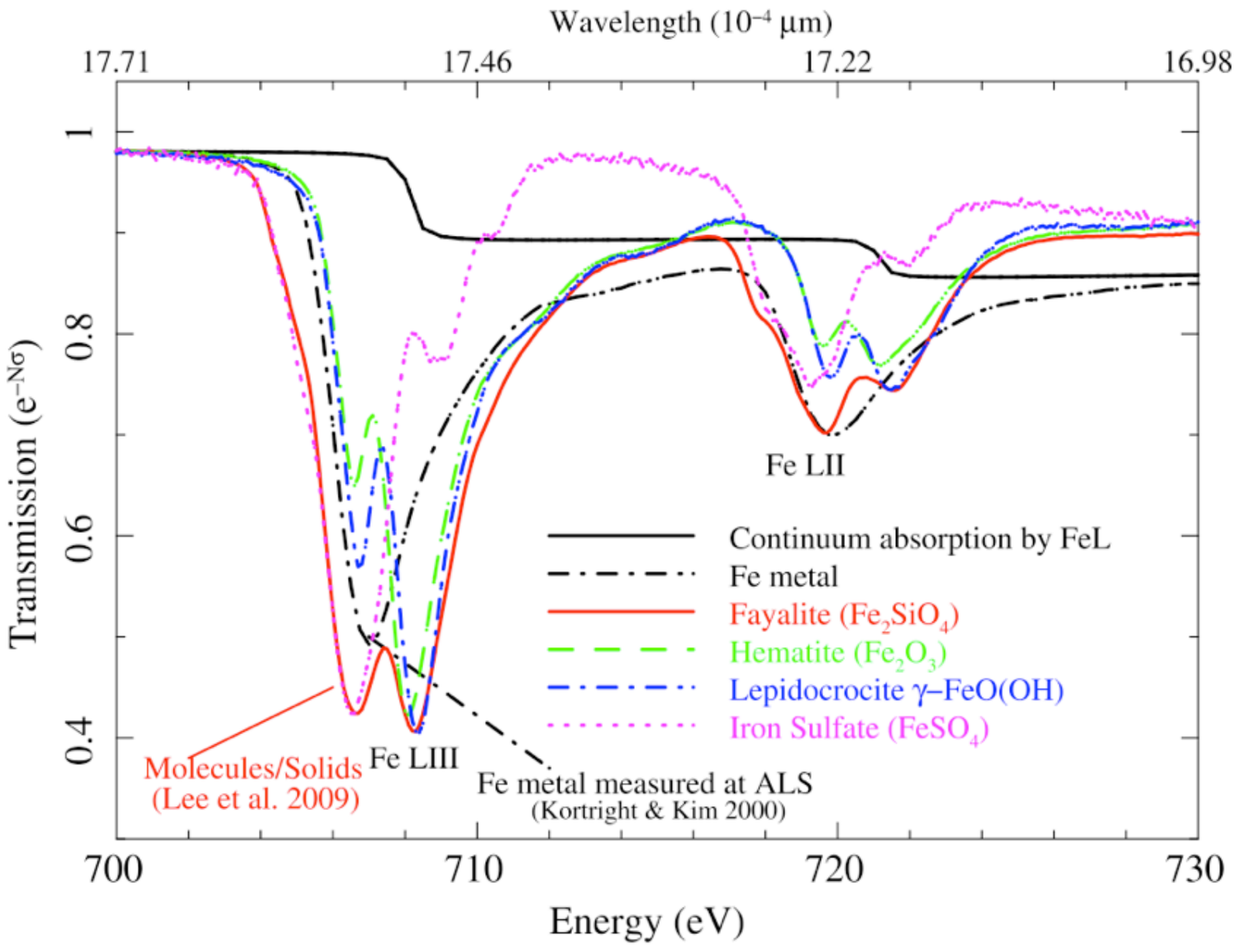


Fig. 1 Absorption calculated from laboratory cross section (σ) measurements for 0.7 keV FeL presented in Lee et al. (2009). At this high spectral resolution ($R = 3000$, the baseline IXO value), different molecules (*color*), metals (*dashed-dot black*) and continuum absorption (*solid black*), are easily distinguished

Julia Lee, *Space Sci. Rev.*, **157,** 93 (2010)

this is still mostly XANES and band structure!

Interstellar Absorption by molecules and dust

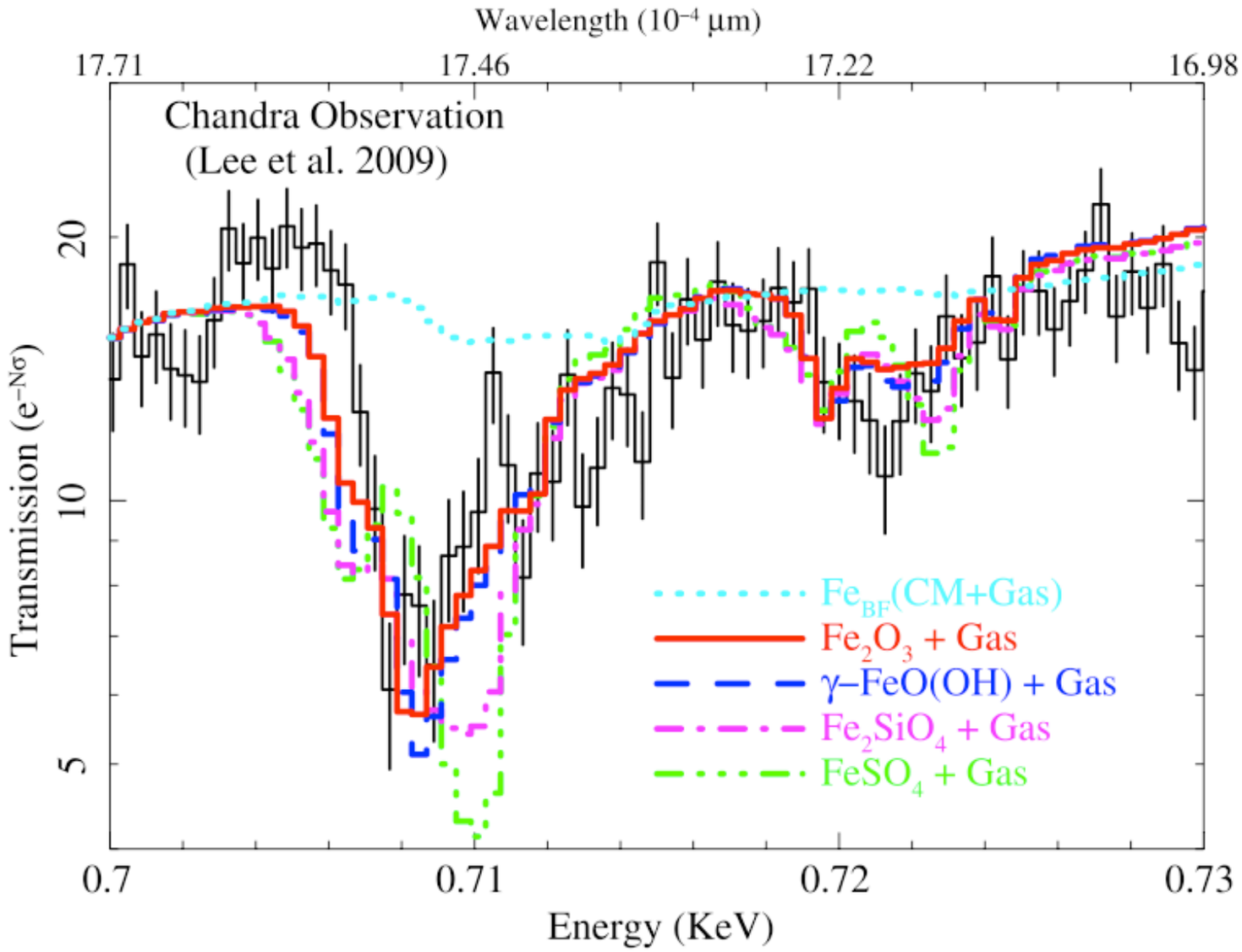
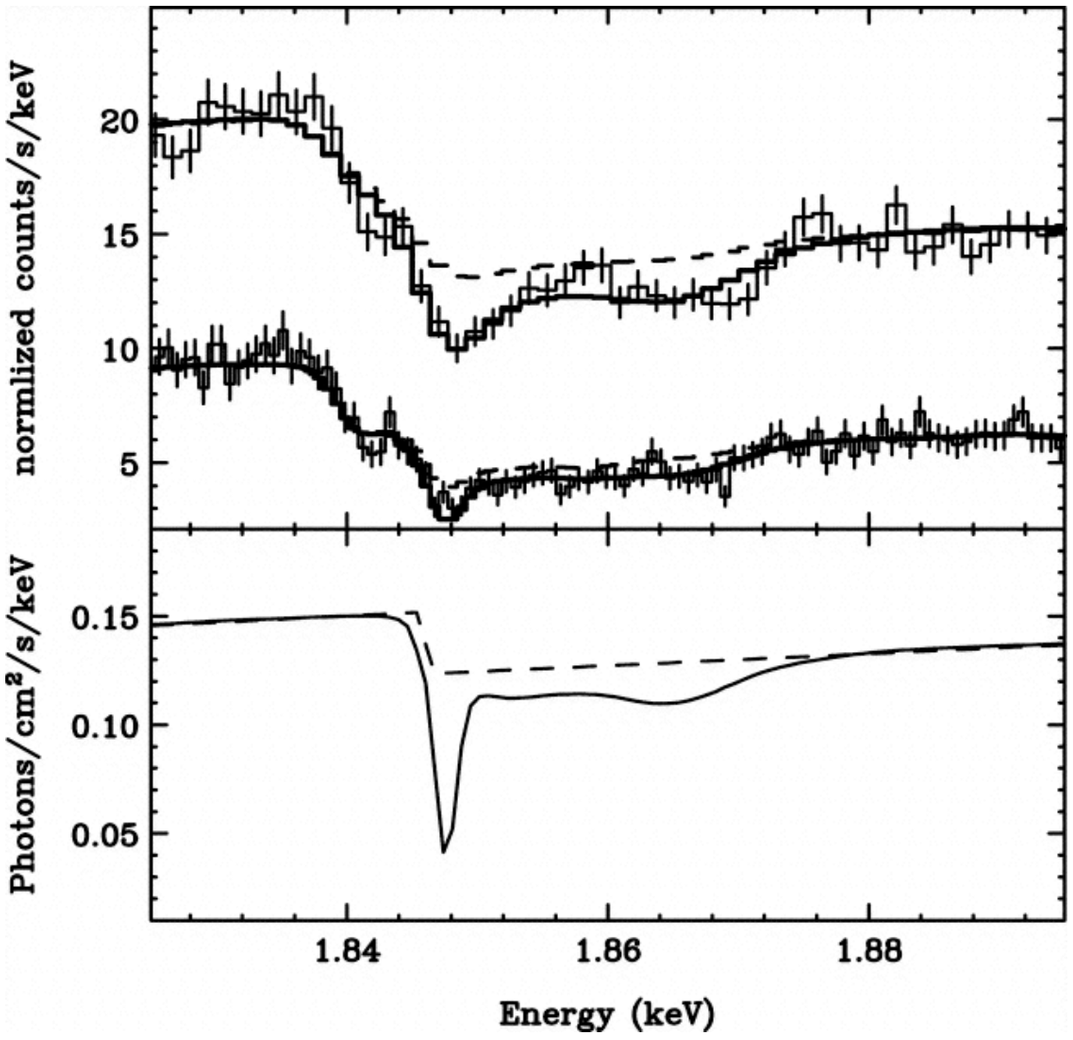


Fig. 2 A 15ks Chandra HETGS observation of Cygnus X-1 (*black*) zoomed in on the ~ 700 eV (~ 17.7 Å) FeL spectral region shows that at the current highest available spectral resolution, we can discern at high confidence between Fe_2O_3 (*red*) and $FeSO_4$ (*green*), but not between e.g. Fe_2O_3 and FeO(OH) (*dark blue*). In *light blue* is continuum absorption by Fe L from both gas and solids (CM). In addition, even for a source as bright as Cyg X-1, a 15 ks integration is require to achieve a S/N ~ 5 per bin. Future missions with higher throughput will allow us to engage in such studies with more sources, and accompanying higher spectral resolution as e.g. that shown in Fig. 1 will enable more involved studies of dust structure, not currently possible

Interstellar Absorption by molecules and dust

real XAFS?

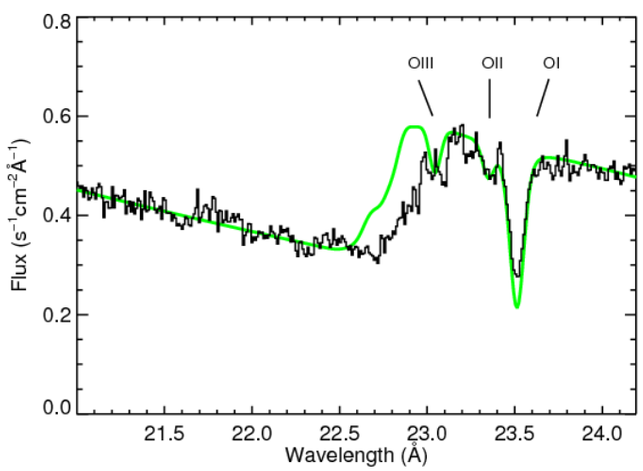


structure at the Si K edge

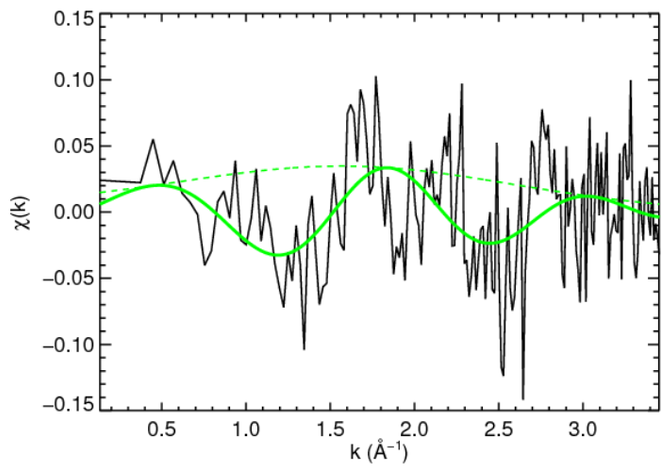
GX 13+1 *Chandra* HETG, METG
Ueda *et al.* 2005
claim: structure not seen in Cyg X-2 (low NH)

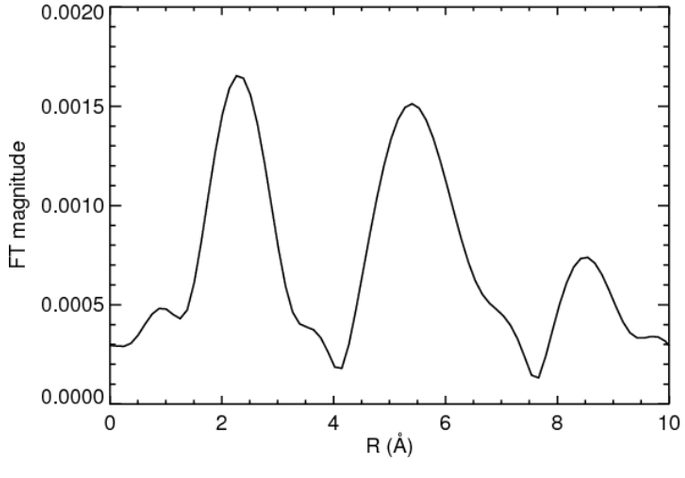
Interstellar Absorption by molecules and dust

real XAFS?



structure at the O K edge
exciting (though puzzling), because consistent with O in water ice!
but signal disappears with use of more sophisticated atomic O cross section...





Sco X-1 *XMM-Newton*/RGS
de Vries & Costantini 2009
modulation at O K