

X-ray spectroscopy

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SRON

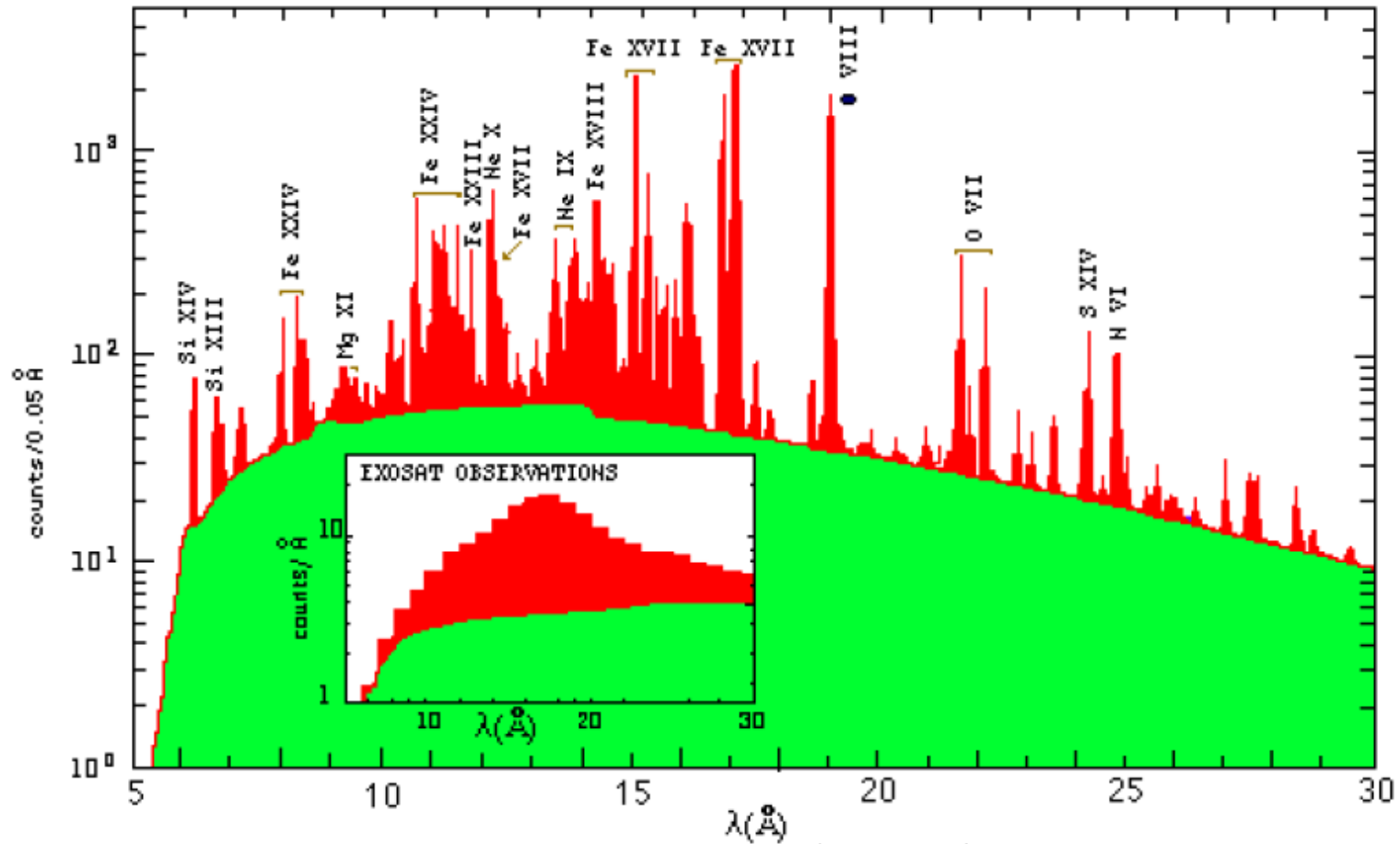


Netherlands Institute for Space Research

Introduction to spectroscopy

The need for high-resolution

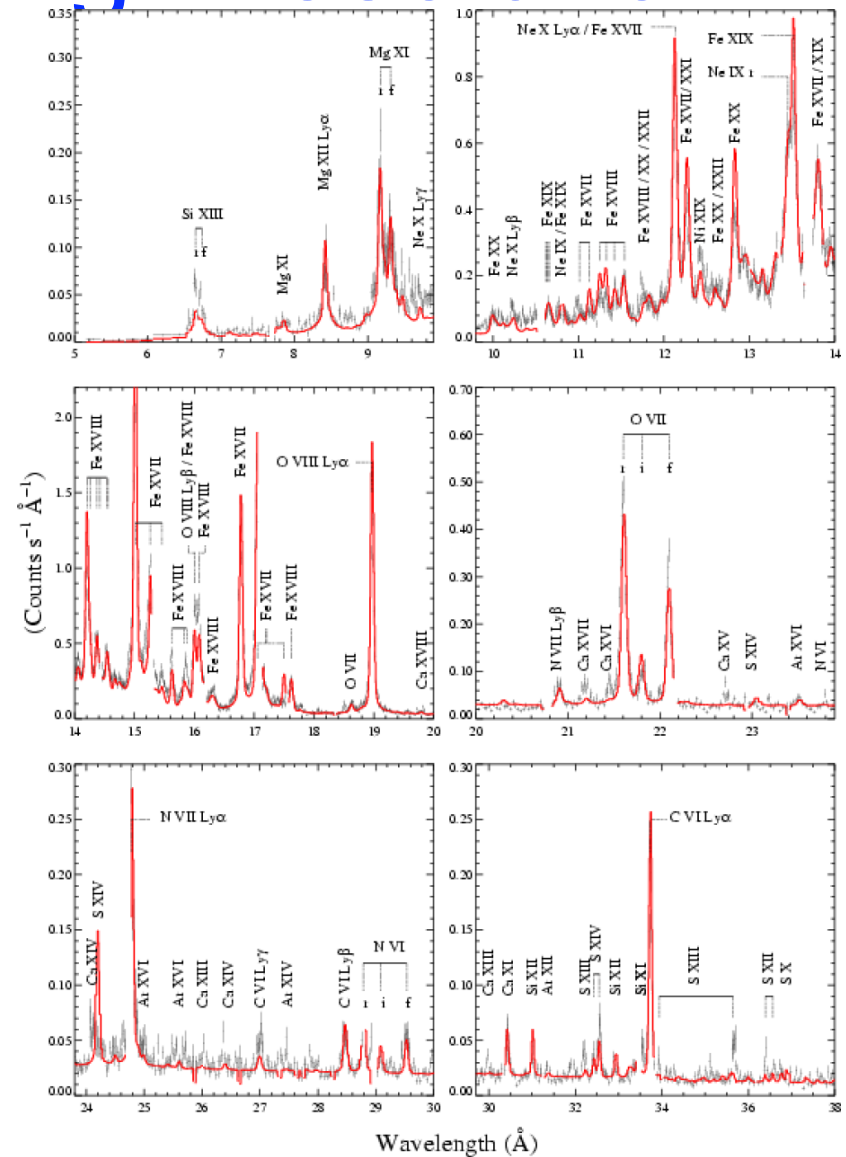
XMM RGS SPECTRUM OF CAPELLA



(Courtesy G. Branduardi-Raymont)

The benefits of high-resolution

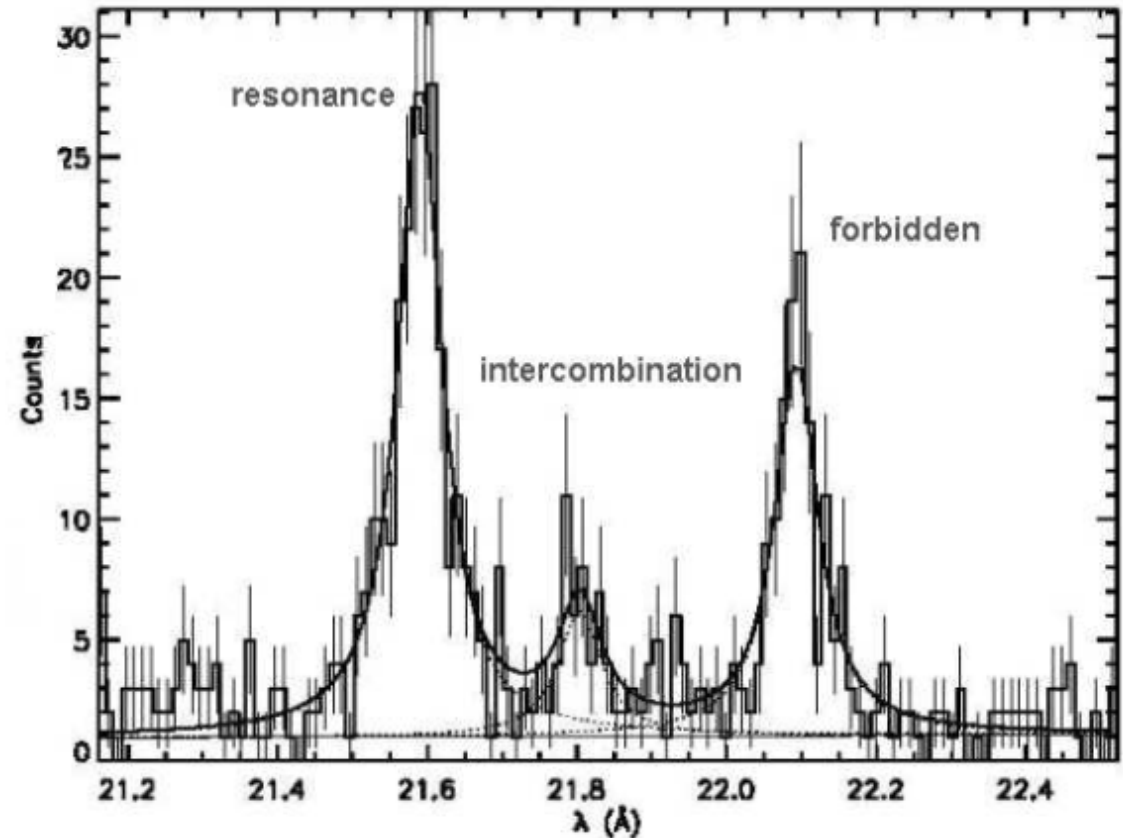
- Wealth of emission lines from different ions, chemical elements over a broad wavelength range



(figure: Capella, Audard et al. 2001)

Line ratios

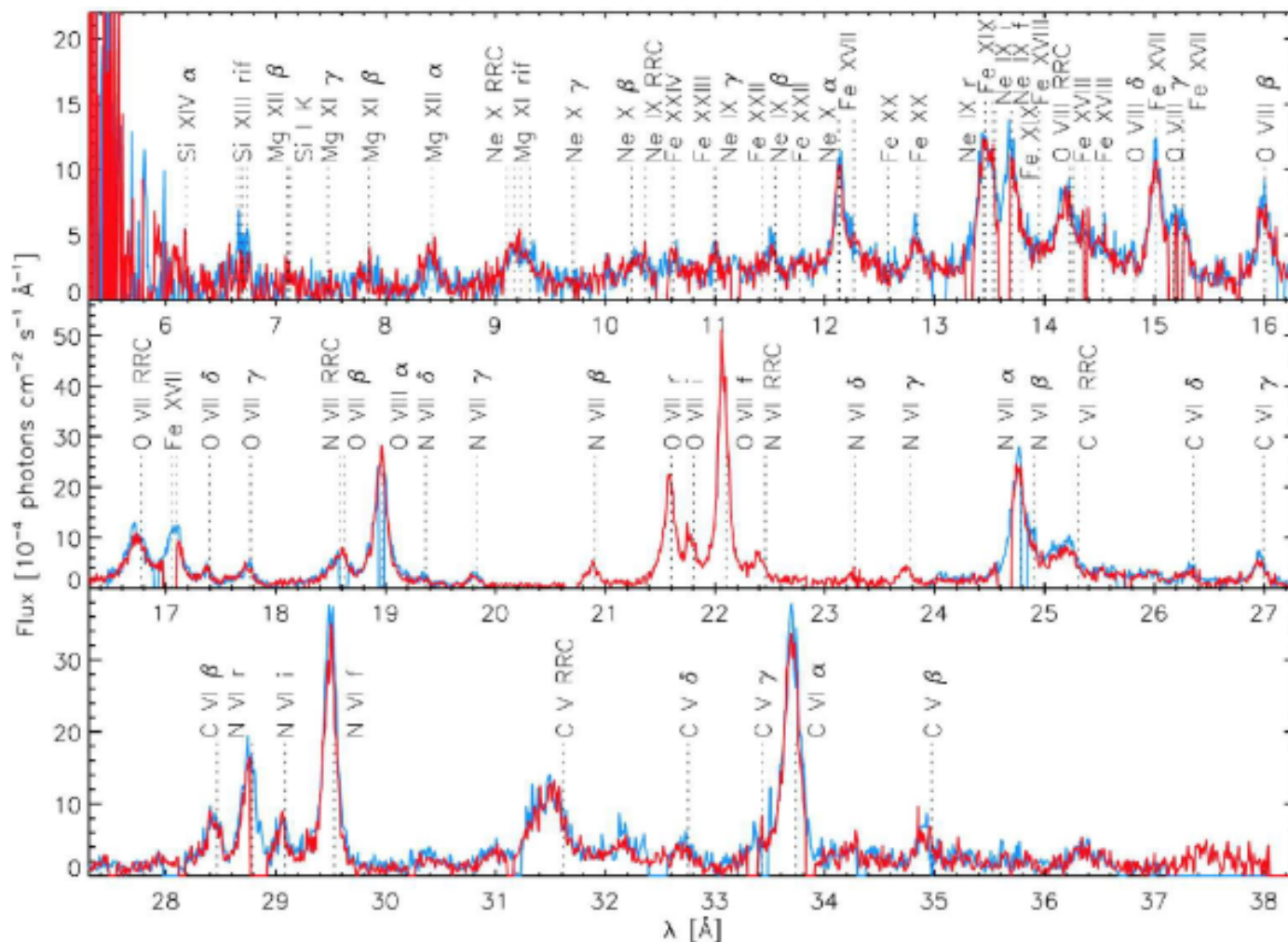
- Line ratios lines from same ion may contain wealth physical info (see later)
- Example: famous O VII triplet



Flare star EQ Peg, courtesy J. Schmitt

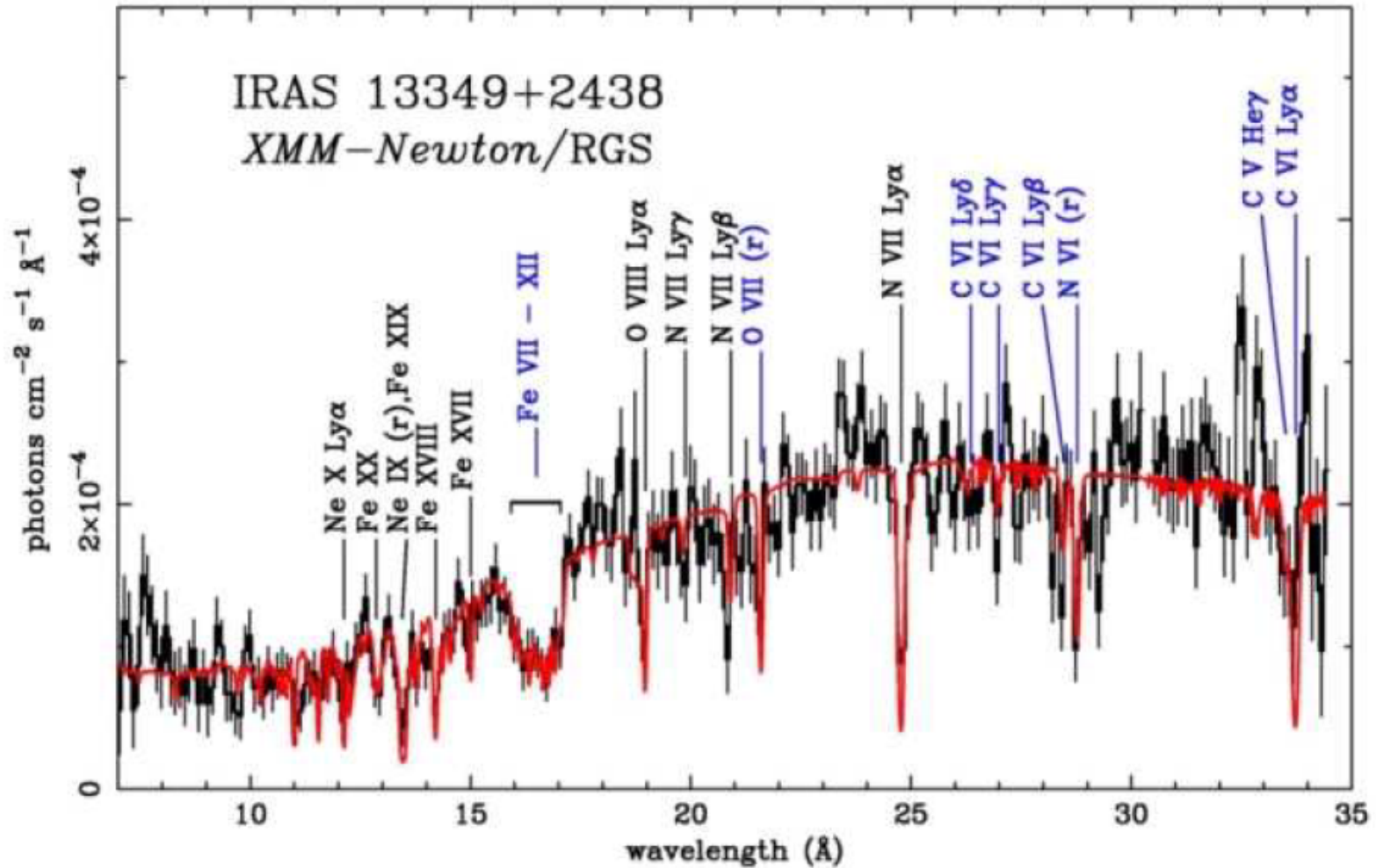
Other sources, same lines: AGN

example: NGC 1068, Seyfert 2, Kinkhabwala et al.2002



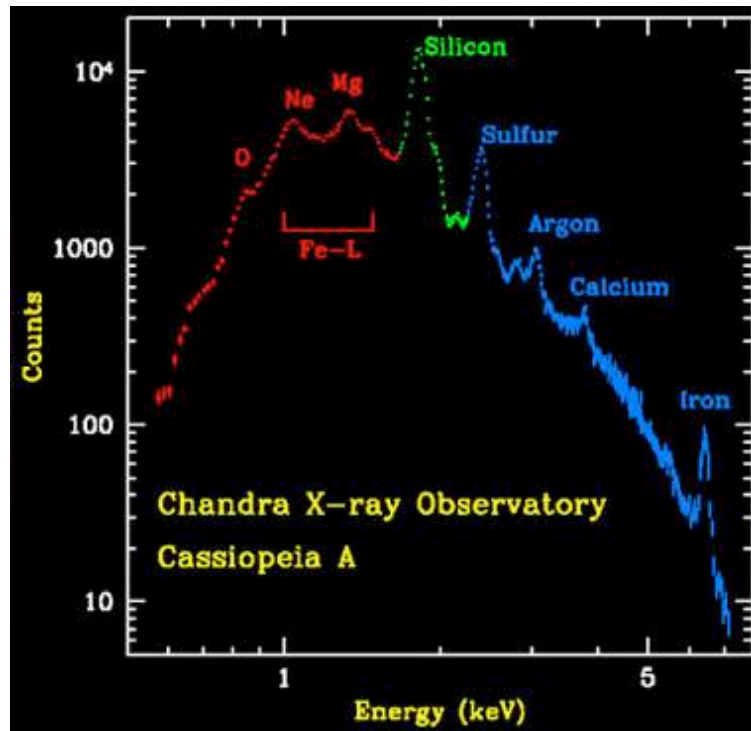
Absorption spectra: same lines, other physics

Example: Sako et al. 2001

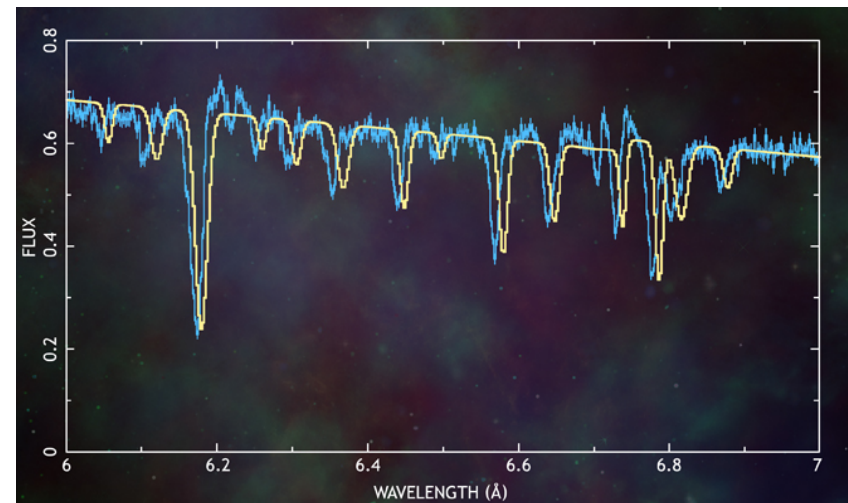


Two types of spectra

Emission



Absorption



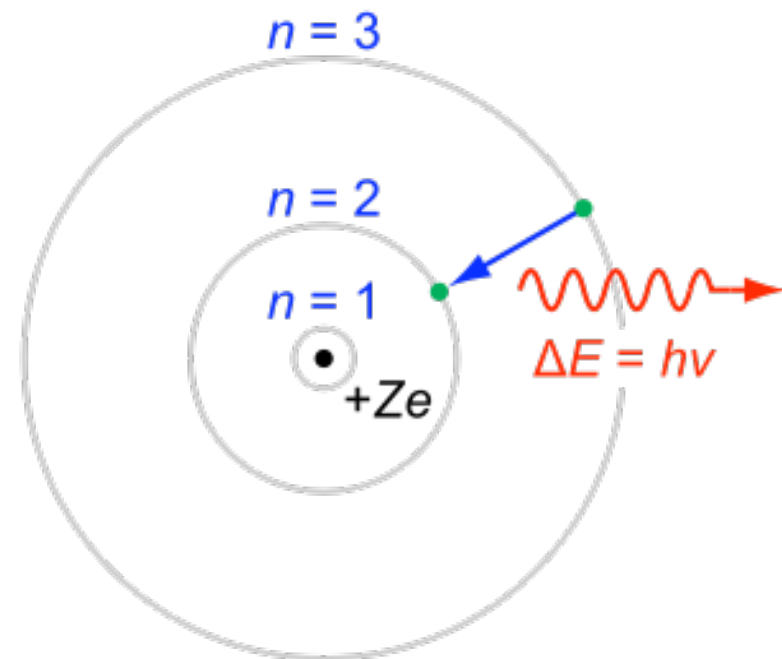
What can you get from a spectrum?

- Electron temperature
- Gas density
- Chemical abundances
- Interstellar dust
- Ion temperature
- Turbulent velocity
- Physical state plasma
- Age plasma
- Volume plasma
- Presence non-thermal electrons

A brief introduction to atomic structure

The Bohr model

- Got this in your quantum class!
- $E_n = -Z^2R/n^2$ with R the Rydberg energy:
- $R = \frac{1}{2} (m_e c^2) \alpha^2 \approx 13.6$ eV with $\alpha \approx 1/137$ the fine structure constant
- For $Z=O(1/\alpha)$ orbital velocities become relativistic



Quantum numbers: single electron

- Four quantum numbers describe electron configuration:
- **n** – principal quantum number (Bohr model) $n=1,2,3,4,\dots$
- **l** – angular momentum orbit; $l=0,1,2,\dots,n-1$;
- **s** – spin electron; $s=\pm\frac{1}{2}$
- **j** – total angular momentum; $|l-s|\leq j\leq |l+s|$

Some common notation

l	$l=0$	$l=1$	$l=2$	$l=3$
Designation	s	p	d	f

- Atomic orbitals indicated by n , l and j as follows:

nl_s

- Examples:

$n=1$ $l=0$ $j=1/2$	$1s_{1/2}$
$n=2$ $l=1$ $j=1/2$	$2p_{1/2}$
$n=2$ $l=1$ $j=3/2$	$2p_{3/2}$

Multi-electron systems

- More than 1 electron: add quantum number according to quantum mechanical rules. See textbooks, e.g. Herzberg 1944
- Notation: use capitals for combined state
- Further same notation as for single electrons:
- $L=0,1,2,3, \dots$ designated by S,P,D,F, ...

Notation for multilevel atom

- Prescribe the *configuration* and the *term*
- Term written as $^{2S+1}L_J$
- Example: a two electron system with one electron in 1s, the other in 2p state, with orbital angular momentum $L=1$, total spin $S=1/2$, and total angular momentum $J=1/2$:



Atomic structure

- The Pauli principle prohibits two electrons to be in the same state → max # electrons in a shell

<i>Shell</i>	<i>Max # electrons</i>
1s	2
2s	2
2p	6
3s	2
3p	6
3d	10
4s	2

Other widely used notation

There is also another notation that is commonly used in X-ray spectroscopy. Shells with $n = 1, 2, 3, 4, 5, 6$ and 7 are indicated with K, L, M, N, O, P, Q. A further subdivision is made starting from low values of ℓ up to higher values of ℓ and from low values of j up to higher values of j :

1s	2s	2p _{1/2}	2p _{3/2}	3s	3p _{1/2}	3p _{3/2}	3d _{3/2}	3d _{5/2}	4s	etc.
K	L _I	L _{II}	L _{III}	M _I	M _{II}	M _{III}	M _{IV}	M _V	N _I	
2	2	2	4	2	2	4	4	6	2	

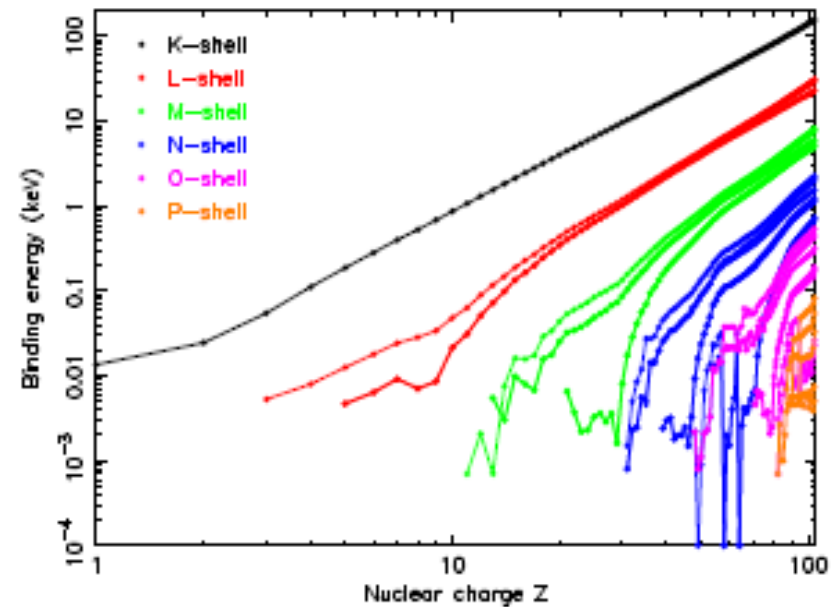
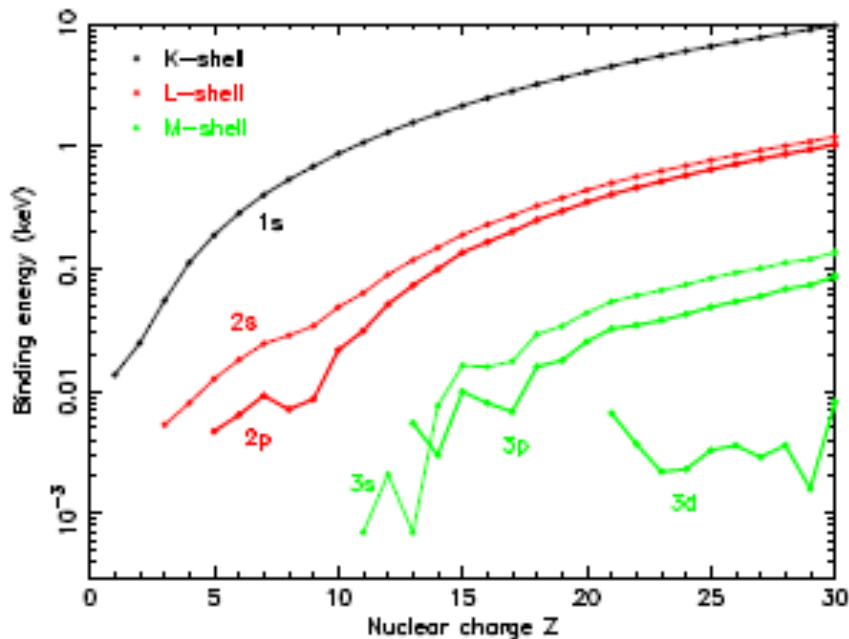
The third row in this table indicates the maximum number of electrons that can be contained in each subshell. This so-called statistical weight is simply $2j + 1$.

The periodic system: atomic structure

Z	El	1s	2s	2p	3s	3p	3d	4s	Ground term
1	H	1							$^2S_{1/2}$
2	He	2							1S_0
3	Li	2	1						$^2S_{1/2}$
4	Be	2	2						1S_0
5	B	2	2	1					$^2P_{1/2}$
6	C	2	2	2					3P_0
7	N	2	2	3					$^4S_{3/2}$
8	O	2	2	4					3P_2
9	F	2	2	5					$^2P_{3/2}$
10	Ne	2	2	6					1S_0
11	Na	2	2	6	1				$^2S_{1/2}$
12	Mg	2	2	6	2				1S_0
13	Al	2	2	6	2	1			$^2P_{1/2}$
14	Si	2	2	6	2	2			3P_0
15	P	2	2	6	2	3			$^4S_{3/2}$

Z	El	1s	2s	2p	3s	3p	3d	4s	Ground term
16	S	2	2	6	2	4			3P_2
17	Cl	2	2	6	2	5			$^2P_{3/2}$
18	Ar	2	2	6	2	6			1S_0
19	K	2	2	6	2	6		1	$^2S_{1/2}$
20	Ca	2	2	6	2	6		2	1S_0
21	Sc	2	2	6	2	6	1	2	$^2D_{3/2}$
22	Ti	2	2	6	2	6	2	2	3F_2
23	V	2	2	6	2	6	3	2	$^4F_{3/2}$
24	Cr	2	2	6	2	6	5	1	7S_3
25	Mn	2	2	6	2	6	5	2	$^6S_{5/2}$
26	Fe	2	2	6	2	6	6	2	5D_4
27	Co	2	2	6	2	6	7	2	$^4F_{9/2}$
28	Ni	2	2	6	2	6	8	2	3F_4
29	Cu	2	2	6	2	6	10	1	$^2S_{1/2}$
30	Zn	2	2	6	2	6	10	2	1S_0

Energy levels free atoms



$E \sim Z^2$ for K-shell
Others more complex due to interactions
Highest E (X-rays!): high Z, inner shells

Energy levels for ions

- Energy levels for ions same element similar, but not the same
- Why?
- Interactions electrons

Ion	E (eV)	λ (Å)
O I	544	22.77
O II	565	21.94
O III	592	20.94
O IV	618	20.06
O V	645	19.22
O VI	671	18.48
O VII	739	16.77
O VIII	871	14.23

Line transitions: selection rules

- If an atom / ion is in **excited** state (higher orbit), it can decay to a lower state by emission of a photon.
- **Required**: initial energy level higher than final energy level
- However, not all transitions allowed (quantum-mechanical **selection rules**)
- Some transitions **forbidden**, but still occur (due to rarer, higher order processes)

Basic processes

Overview of processes

a) Radiative transitions

b) Excitation processes

1. Collisional excitation
2. Collisional de-excitation
3. Radiative excitation

c) Auger processes & fluorescence

d) Bremsstrahlung

e) Two photon emission

f) Ionisation processes

1. Collisional (direct) ionisation
2. Excitation- autoionisation
3. Photoionisation
4. Compton ionisation

g) Recombination processes

1. Radiative recombination
2. Dielectronic recombination

h) Charge transfer processes

1. Charge transfer ionisation
2. Charge transfer recombination

Spontaneous emission

- An atom in an excited state k can decay to a lower state i by emitting a photon. The probability per unit time is A_{ik} (s^{-1}).
- Depending on the available energy levels & selection rules, state k may decay also to other levels (*branching*)
- If the transition is not to the ground state, more transitions may follow (*cascade*)

Collisional excitation

The cross section Q_{ij} for excitation from level i to level j for this process can be conveniently parametrised by

$$Q_{ij}(U) = \frac{\pi a_0^2}{w_i} \frac{E_H}{E_{ij}} \frac{\Omega(U)}{U}, \quad (3.3)$$

where $U = E/E_{ij}$ with E_{ij} the excitation energy from level i to j , E the energy of the exciting electron, E_H the Rydberg energy (13.6 eV), a_0 the Bohr radius and w_i the statistical weight of the lower level i . The dimensionless quantity $\Omega(U)$ is the so-called collision strength. For a given transition on an iso-electronic sequence, $\Omega(U)$ is not a strong function of the atomic number Z , or may be even almost independent of Z .

Mewe (1972) introduced a convenient formula that can be used to describe most collision strengths, written here as follows:

$$\Omega(U) = A + \frac{B}{U} + \frac{C}{U^2} + \frac{2D}{U^3} + F \ln U, \quad (3.4)$$

where A , B , C , D and F are parameters that differ for each transition. The expression can be integrated analytically over a Maxwellian electron distribution, and the result can be expressed in terms of exponential integrals.

Collisional excitation II

- Rates (m^3/s) can be calculated averaging over a Maxwellian; asymptotics:

$$kT \ll E_{ij}, y \gg 1 : S_{ij} \simeq S_0(A + B + C + 2D)T^{-\frac{1}{2}}e^{-E_{ij}/kT} \quad (3.15)$$

$$kT \gg E_{ij}, y \ll 1 : S_{ij} \simeq S_0FT^{-\frac{1}{2}} \ln(kT/E_{ij}) \quad (3.16)$$

For low T there are exponentially few excitations (only the tail of the Maxwellian has sufficient energy for excitation); for high T the number of excitations also approaches zero, because of the small collision cross section.

Collisional de-excitation

- Inverse process of collisional excitation: collision by a free electron can bring bound electron into higher level
- Sometimes only way to get electron back to ground state, when no radiative transitions are allowed → density dependence of spectral lines

Radiative excitation (line absorption)

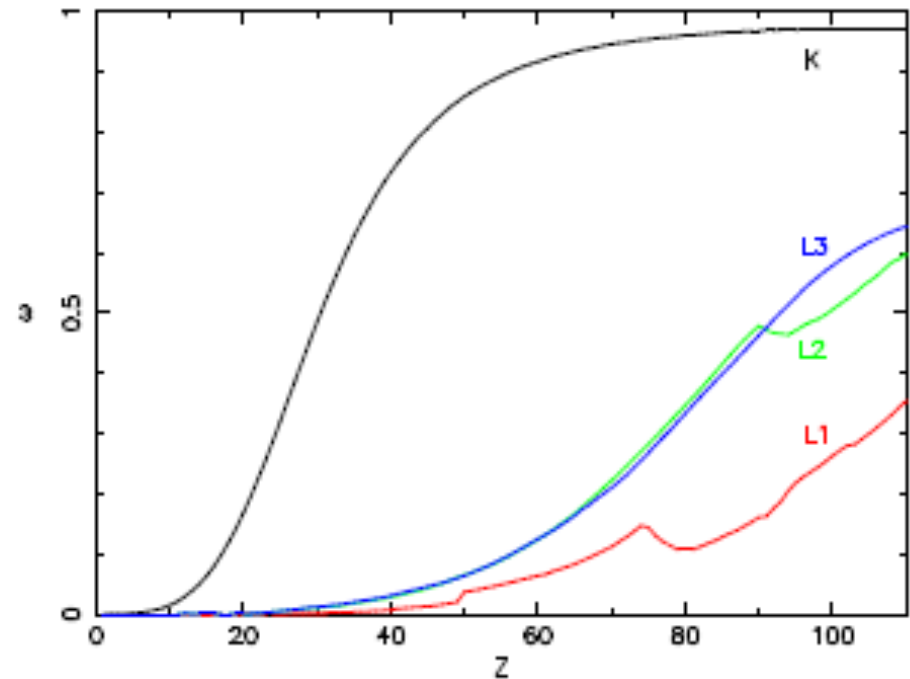
- Photon encounter with ion: photon can be absorbed → ion in excited state
- When ion de-excites afterwards by emitting photon of same energy, process is called resonance scattering

$$\tau_0 = \frac{\alpha h \lambda f N_i}{2\sqrt{2\pi} m_e \sigma_v}. \quad (44)$$

Apart from the fine structure constant α and Planck's constant h , the optical depth also depends on the properties of the absorber, namely the ionic column density N_i and the velocity dispersion σ_v . Furthermore, it depends on the oscillator strength f which is a dimensionless quantity that is different for each transition and is of order unity for the strongest transitions.

Fluorescence

- Create a hole in electron distribution by ionisation (through photons, electrons)
- Hole filled by electron from higher shell
- Result: photon compensating energy difference
- Efficiency: fluorescence rate ω depends on nuclear charge Z



Dictionary of inner-shell transitions

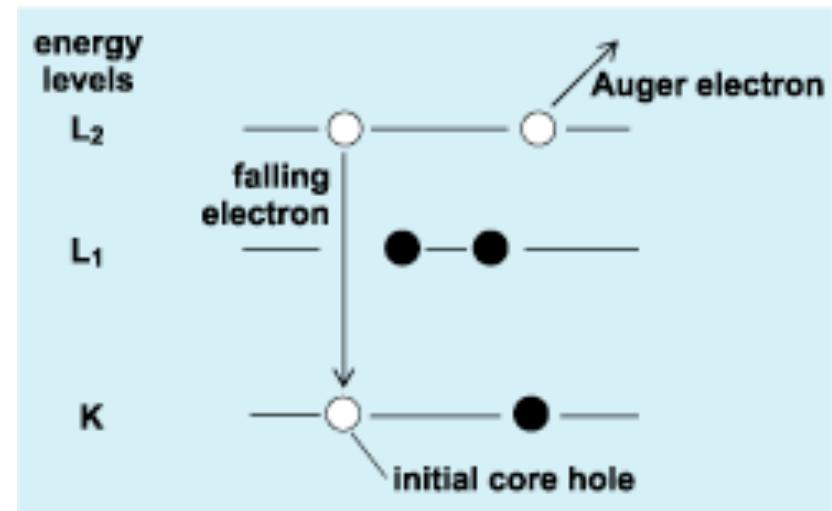
(once you encounter them;

IUPAC = International Union of Pure and Applied Chemistry)

Siegbahn	IUPAC	Siegbahn	IUPAC	Siegbahn	IUPAC	Siegbahn	IUPAC
$K\alpha_1$	K-L ₃	$L\alpha_1$	L ₃ -M ₅	$L\gamma_1$	L ₂ -N ₄	$M\alpha_1$	M ₅ -N ₇
$K\alpha_2$	K-L ₂	$L\alpha_2$	L ₃ -M ₄	$L\gamma_2$	L ₁ -N ₂	$M\alpha_2$	M ₅ -N ₆
$K\beta_1$	K-M ₃	$L\beta_1$	L ₂ -M ₄	$L\gamma_3$	L ₁ -N ₃	$M\beta$	M ₄ -N ₆
$K^I\beta_2$	K-N ₃	$L\beta_2$	L ₃ -N ₅	$L\gamma_4$	L ₁ -O ₃	$M\gamma$	M ₃ -N ₅
$K^{II}\beta_2$	K-N ₂	$L\beta_3$	L ₁ -M ₃	$L\gamma'_4$	L ₁ -O ₂	$M\zeta$	M _{4,5} -N _{2,3}
$K\beta_3$	K-M ₂	$L\beta_4$	L ₁ -M ₂	$L\gamma_5$	L ₂ -N ₁		
$K^I\beta_4$	K-N ₅	$L\beta_5$	L ₃ -O _{4,5}	$L\gamma_6$	L ₂ -O ₄		
$K^{II}\beta_4$	K-N ₄	$L\beta_6$	L ₃ -N ₁	$L\gamma_8$	L ₂ -O ₁		
$K\beta_{4x}$	K-N ₄	$L\beta_7$	L ₃ -O ₁	$L\gamma'_8$	L ₂ -N ₆₍₇₎		
$K^I\beta_5$	K-M ₅	$L\beta'_7$	L ₃ -N _{6,7}	$L\eta$	L ₂ -M ₁		
$K^{II}\beta_5$	K-M ₄	$L\beta_9$	L ₁ -M ₅	$L\ell$	L ₃ -M ₁		
		$L\beta_{10}$	L ₁ -M ₄	Ls	L ₃ -M ₃		
		$L\beta_{15}$	L ₃ -N ₄	Lt	L ₃ -M ₂		
		$L\beta_{17}$	L ₂ -M ₃	Lu	L ₃ -N _{6,7}		
				Lv	L ₂ -N ₆₍₇₎		

Auger processes (Autoionisation)

- Create hole in electron distribution by ionisation (through photons, electrons)
- Fill hole without emitting photons: one electron falls, but other is ejected



Bremsstrahlung

Bremsstrahlung is caused by a collision between a free electron and an ion. The emissivity ϵ_{ff} (photons $\text{m}^{-3} \text{s}^{-1} \text{J}^{-1}$) can be written as:

$$\epsilon_{\text{ff}} = \frac{2\sqrt{2}\alpha\sigma_{\text{T}}cn_en_iZ_{\text{eff}}^2}{\sqrt{3\pi}E} \left(\frac{m_e c^2}{kT}\right)^{\frac{1}{2}} g_{\text{ff}} e^{-E/kT},$$

where α is the fine structure constant, σ_{T} the Thomson cross section, n_e and n_i the electron and ion density, and E the energy of the emitted photon. The factor g_{ff} is the so-called Gaunt factor and is a dimensionless quantity of order unity. Further, Z_{eff} is the effective charge of the ion, defined as

$$Z_{\text{eff}} = \left(\frac{n_r^2 I_r}{E_{\text{H}}}\right)^{\frac{1}{2}}$$

where E_{H} is the ionisation energy of hydrogen (13.6 eV), I_r the ionisation potential of the ion after a recombination, and n_r the corresponding principal quantum number.

Bremsstrahlung II

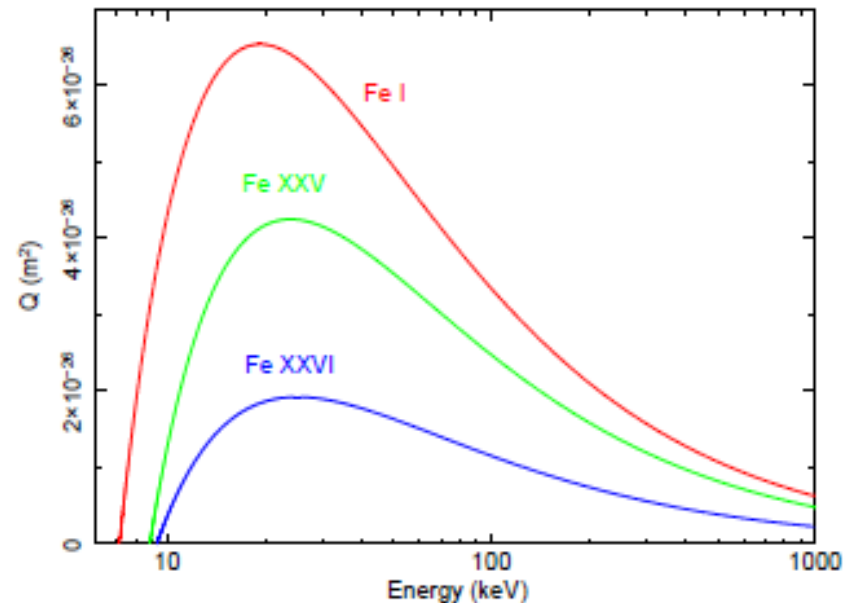
- Spectrum has exponential cut-off at $E=kT$
- Need to add contributions from all ions in the plasma (not just hydrogen!)

Two photon emission

- Important for H-like or He-like ions
- Happens after collisional excitation $1s \rightarrow 2s$
- No radiative way back to 1s (not allowed)
- Has to stay there forever (waiting for collisional excitation to higher level & subsequent decay)
- But rare process may occur: submitting two photons simultaneously; sum energies equals 1s-2p energy difference; further no constraint
- \rightarrow effectively continuum emission process, though formally double line emission

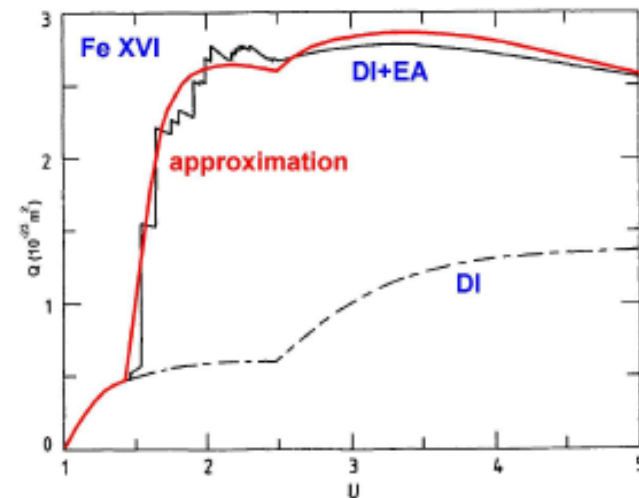
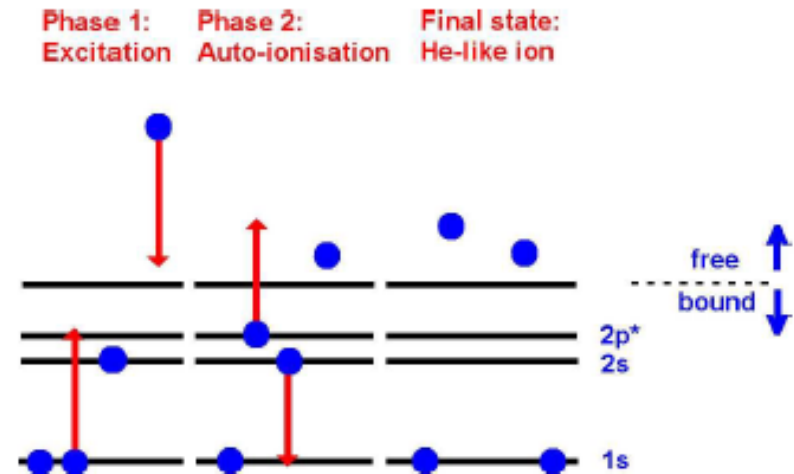
Collisional ionisation

- Free electron kicks out bound electron
- Kinetic energy free electron > ionisation potential
- Cross section smaller at high E
- Average cross section over Maxwellian to get rates
- Contributions from all shells; usually (but not always) mostly the outer shells



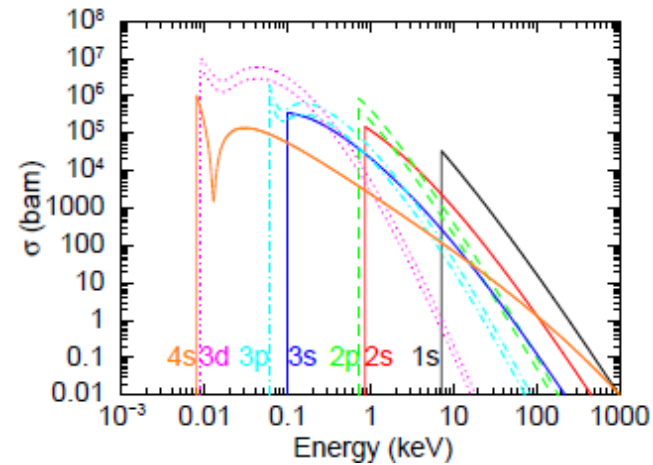
Excitation-Autoionisation

- Two stage process:
- Free electron excites the ion
- Ion decays through autoionisation
- Important for some sequences such as Li-like, Na-like ions
- Example: Li-like ion

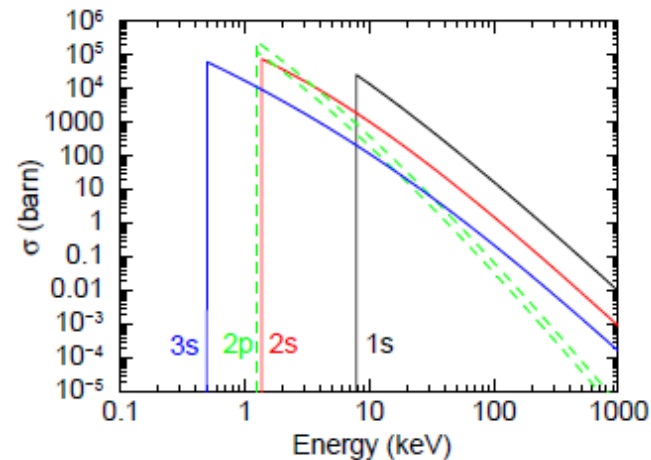


Photoionisation

- Photo-electric effect: photon kicks out electron
- Photon energy > ionisation potential shell
- Cross section >0 @ threshold
- @ fixed E, stronger for inner shells
- Cooper minima
- Edges @ higher E for more highly ionised ions
- K-shell: cross section $\sigma \sim E^{-3}$ → incoming spectrum just above the edge most important



Fe I

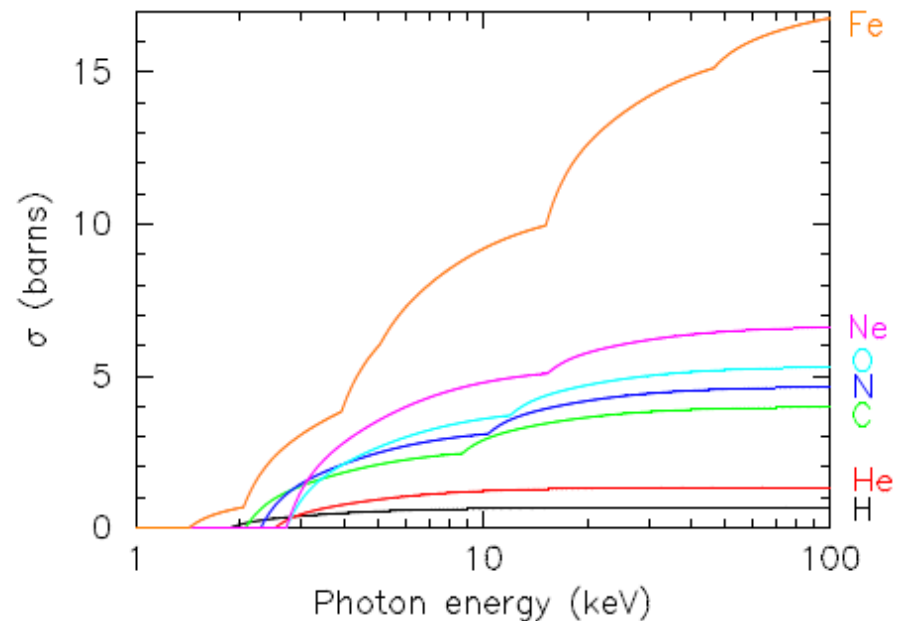


Fe XVI

Compton ionisation

- Compton scattering photon on free electron well known
- Process also works on bound electrons
- @ high E more important than photoionisation
- Threshold energy:

$$E \simeq \sqrt{Im_e c^2 / 2} \gg I$$



Radiative recombination

- Inverse process of photoionisation: free electron captured in bound orbit
- Cross-section proportional to photoionisation cross section
- Recombination rate obtained by integration over Maxwellian
- Asymptotics:

$$kT \ll I : R_n \sim T^{-\frac{1}{2}}$$

$$kT \gg I : R_n \sim \ln(I/kT)T^{-3/2}$$

Radiative recombination II

- Why *radiative* recombination?
- Energy conservation → a photon must be emitted carrying energy loss captured electron
- $E_{\text{photon}} > I$ → low-E threshold, continuum emission
- If electron captured in higher orbit, further decay by line radiation possible
- $kT \ll I$ (recombining plasma): capture into many levels
- $kT \gg I$ (ionising plasma): capture mainly to ground & low-lying levels

Dielectronic recombination

- Inverse process of excitation-autoionisation:
- Free electron captured into higher orbit $(nl)''$, while @ same time electron from lower level is excited to higher level $(nl)'$ → *doubly excited state*
- Usually followed by autoionisation, but one electron (e.g. $(nl)'$) may decay radiatively
- Energy emission line slightly different from "normal" line due to presence "spectator" electron $(nl)''$
- Finally spectator electron may also decay → multiple photon emission
- Due to large number combinations $(nl)''$ and $(nl)'$, complex to calculate

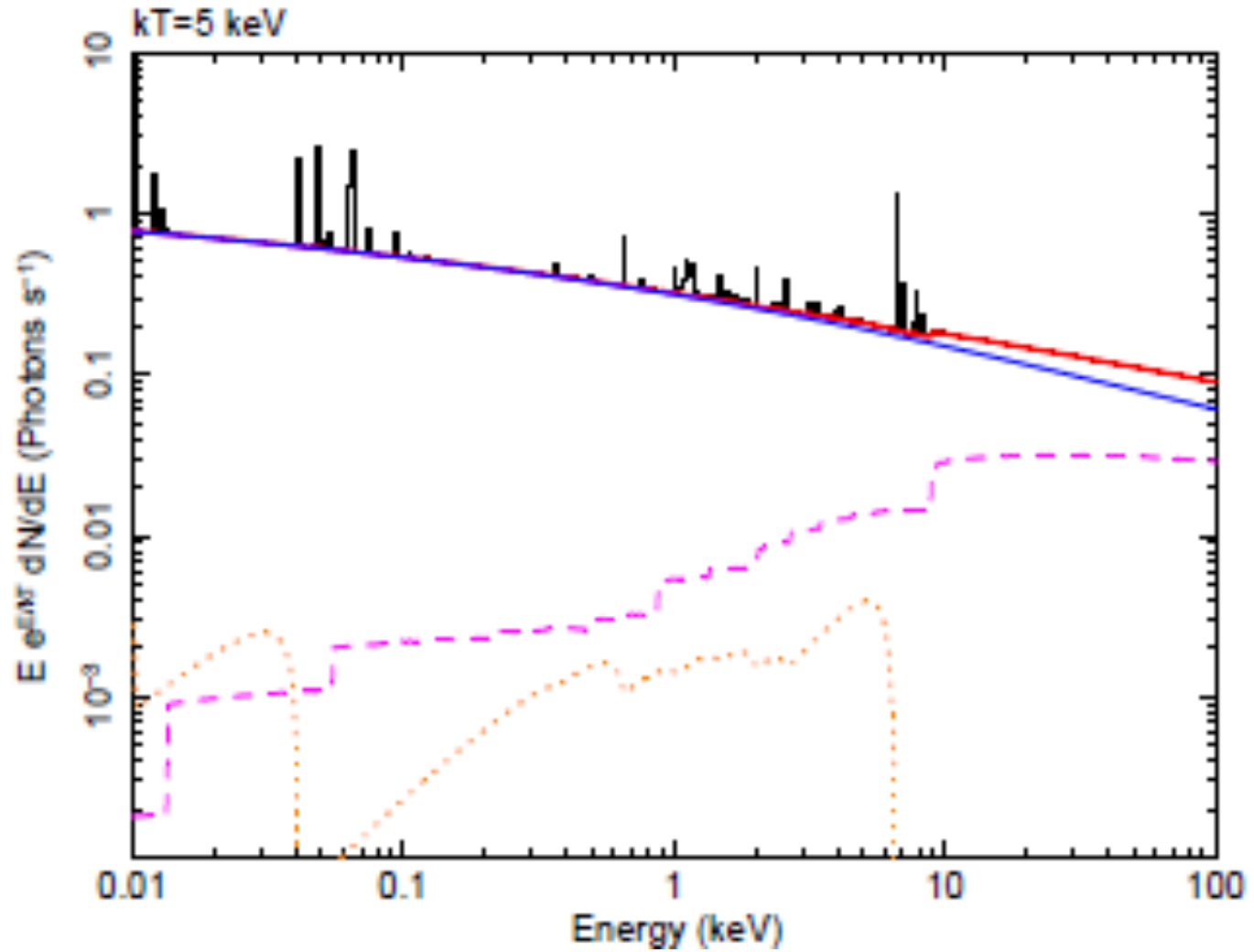
Charge transfer processes

- Ions may exchange an electron:
- Recombination: $\text{H} + \text{O}^{8+} \rightarrow \text{H}^+ + \text{O}^{7+}$
- Ionisation: inverse process
- Due to high abundance H & He, for metals ($Z > 2$) mostly interactions with H or He ions important
- Usually associated emission lines, but due to energy conservation often dominance higher-order lines (e.g. Lyman δ of O VIII enhanced)

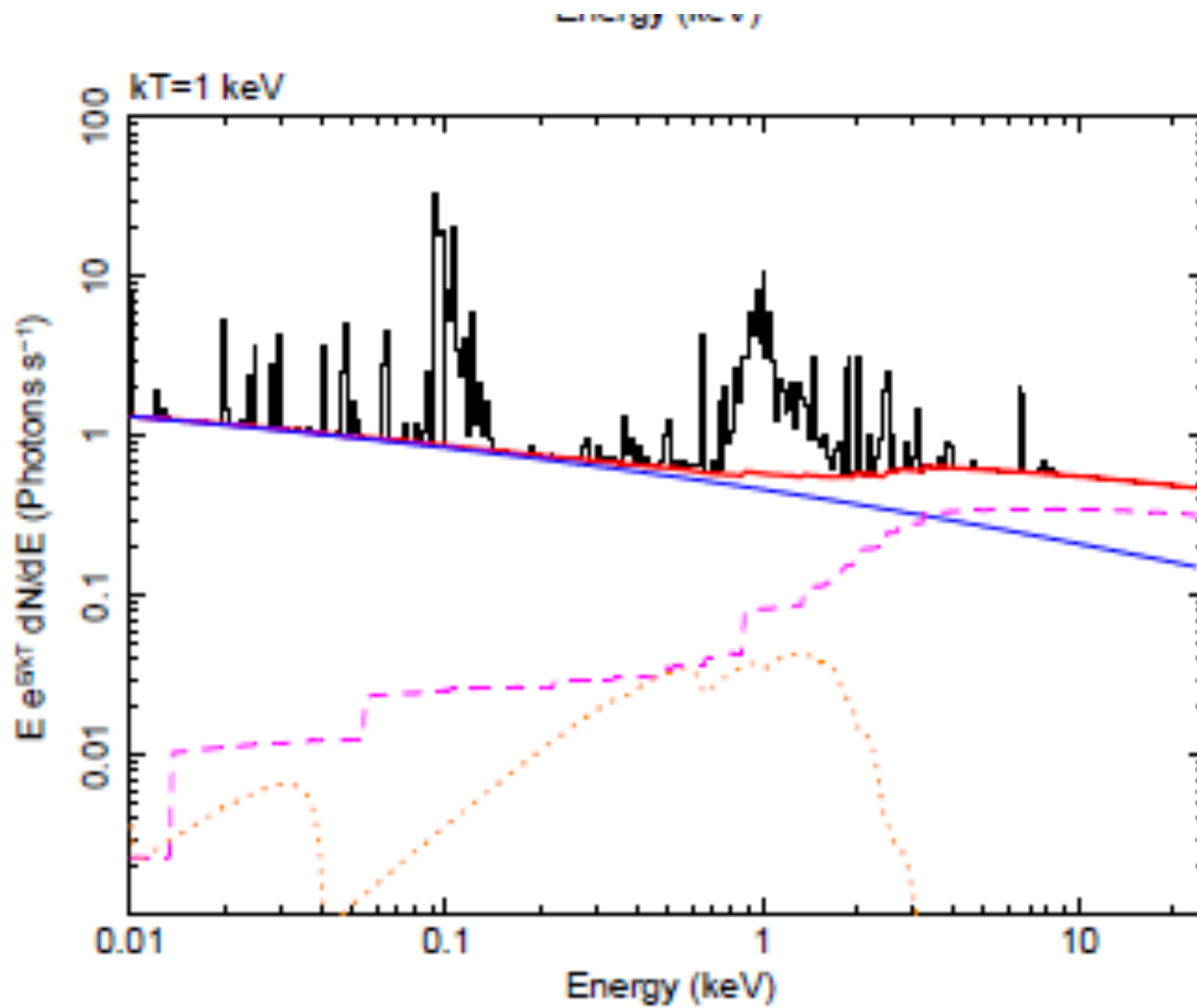
Emission spectrum

- *Continuum emission components*
 - Bremsstrahlung
 - Radiative Recombination Continuum
 - Two photon emission
- *Line emission components*
 - Collisional excitation
 - Radiative recombination
 - Dielectronic recombination
 - Dielectronic satellites
 - Inner shell ionisation

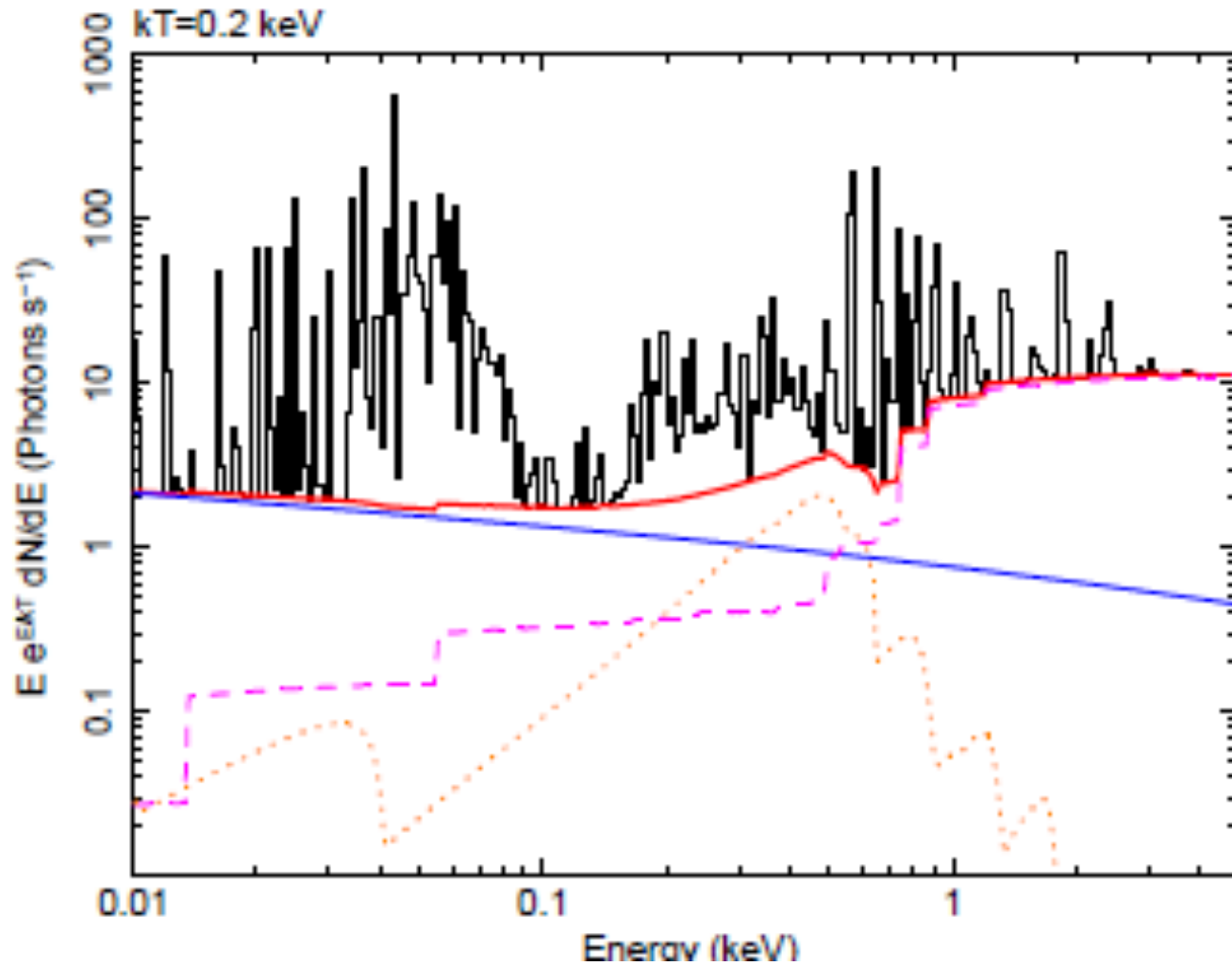
CIE spectrum



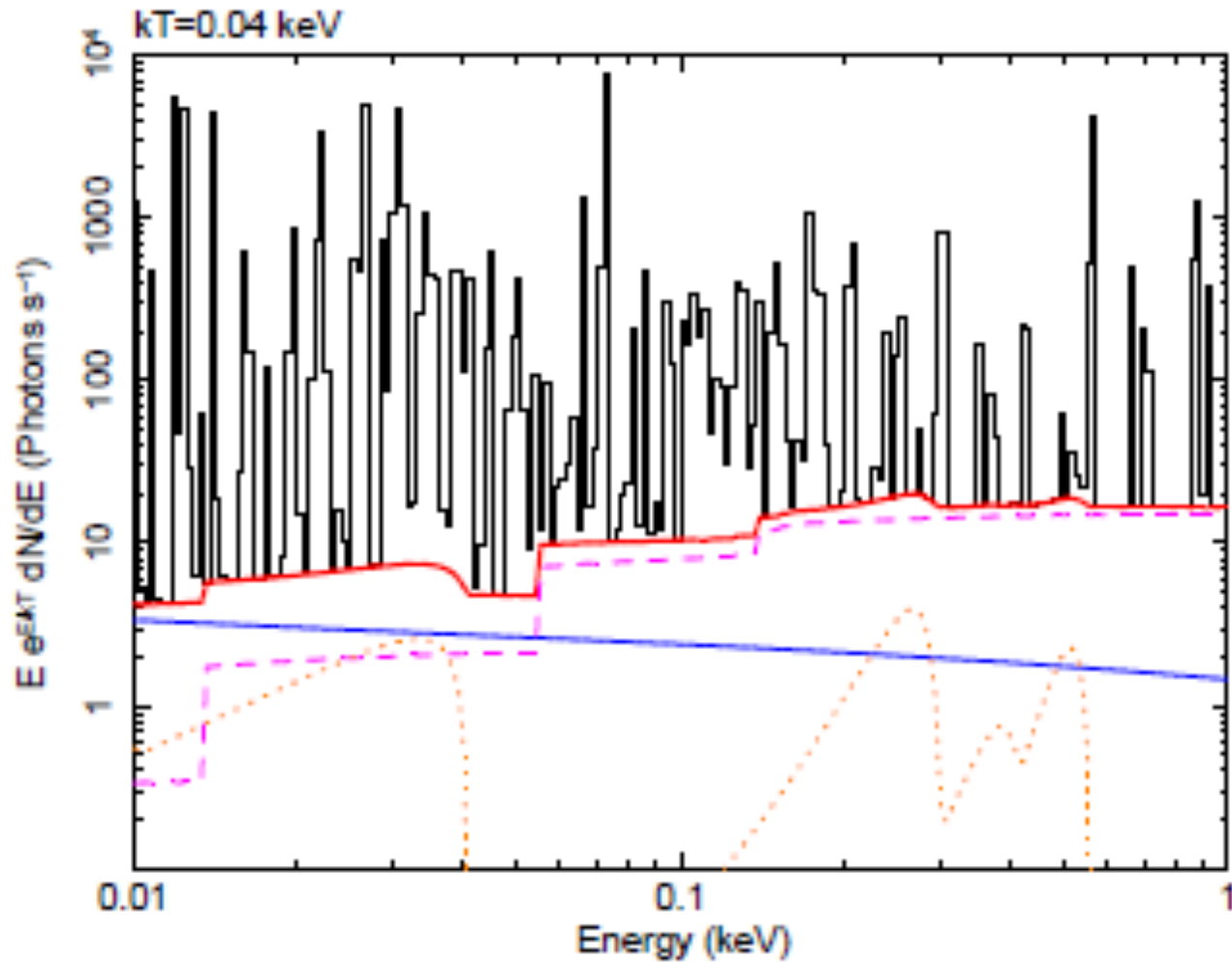
CIE spectrum



CIE spectrum



CIE spectrum



Ionisation (non)equilibrium

Ionisation equilibrium

In equilibrium, ions ionise & recombine continuously, but **no** net change in concentrations

- Simplest case: *collisional ionisation equilibrium (CIE)*
- More complex: *photoionisation equilibrium (PIE)*
- Time-dependent plasma: *non-equilibrium ionisation (NEI)*

Collisional ionisation equilibrium (CIE)

- Only collisional processes (no strong radiation field)

We define R_z as the total recombination rate of an ion with charge z to charge $z-1$, and I_z as the total ionisation rate for charge z to $z+1$. Ionisation equilibrium then implies that the net change of ion concentrations n_z should be zero:

$$z > 0: \quad n_{z+1}R_{z+1} - n_zR_z + n_{z-1}I_{z-1} - n_zI_z = 0$$

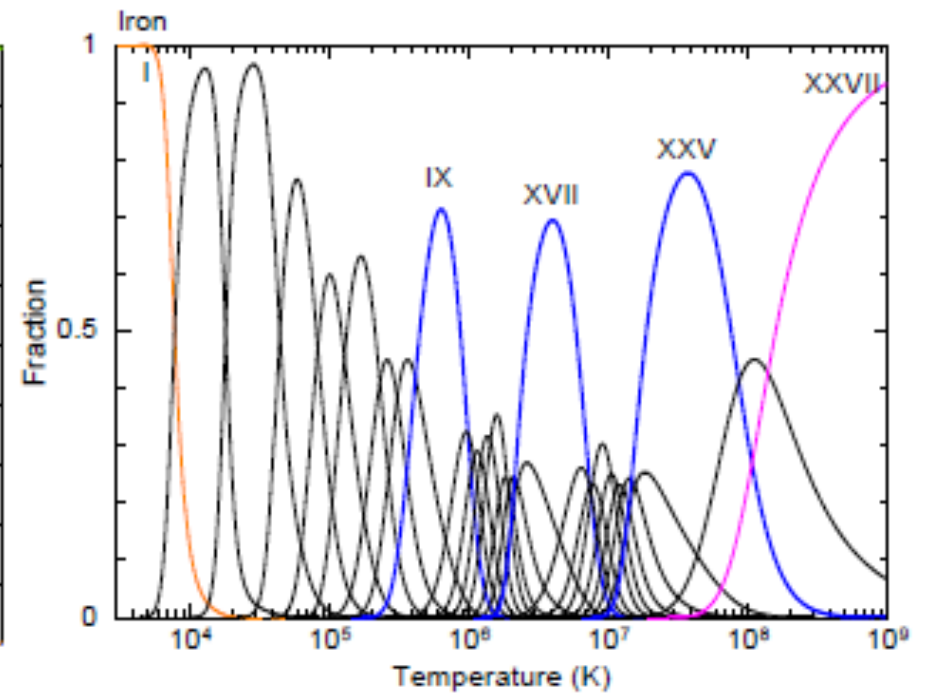
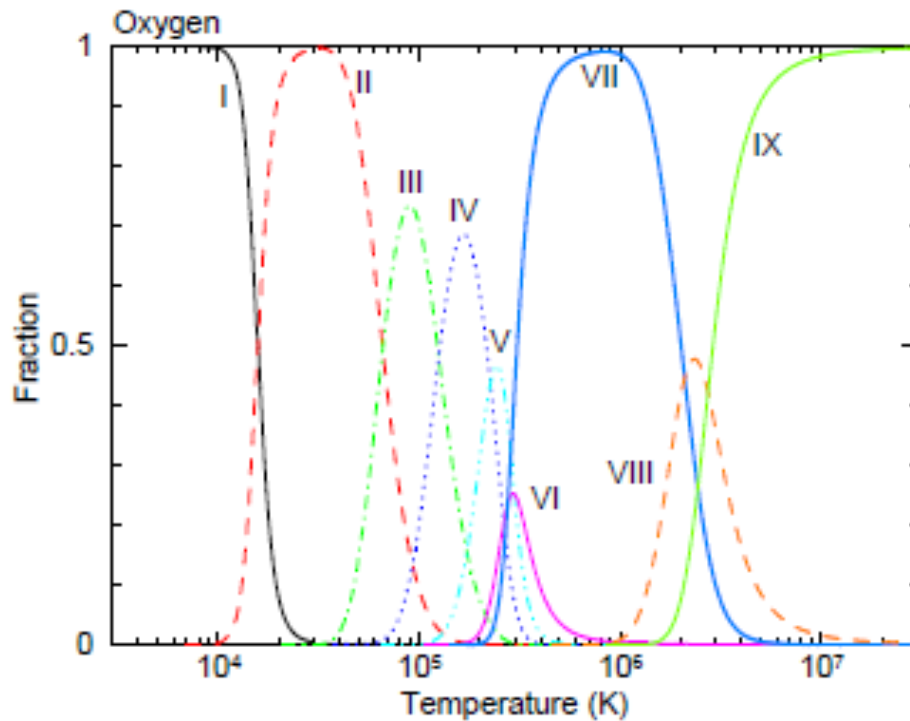
and in particular for $z = 0$ one has

$$n_1R_1 = n_0I_0$$

(a neutral atom cannot recombine further and it cannot be created by ionisation).

Solution depends only on temperature T :
through $R(T)$ and $I(T)$

Example of equilibrium concentrations



Photoionisation equilibrium (PIE)

- Extension of CIE model: all ionisation and recombination processes taken into account
- Solution depends both on T and *radiation field*
- Needs to solve two equations: *ionisation balance* as before and *energy balance* (heating=cooling, where both terms contain several processes)
- Most important balancing processes often photoionisation and collisional recombination (radiative, dielectronic)

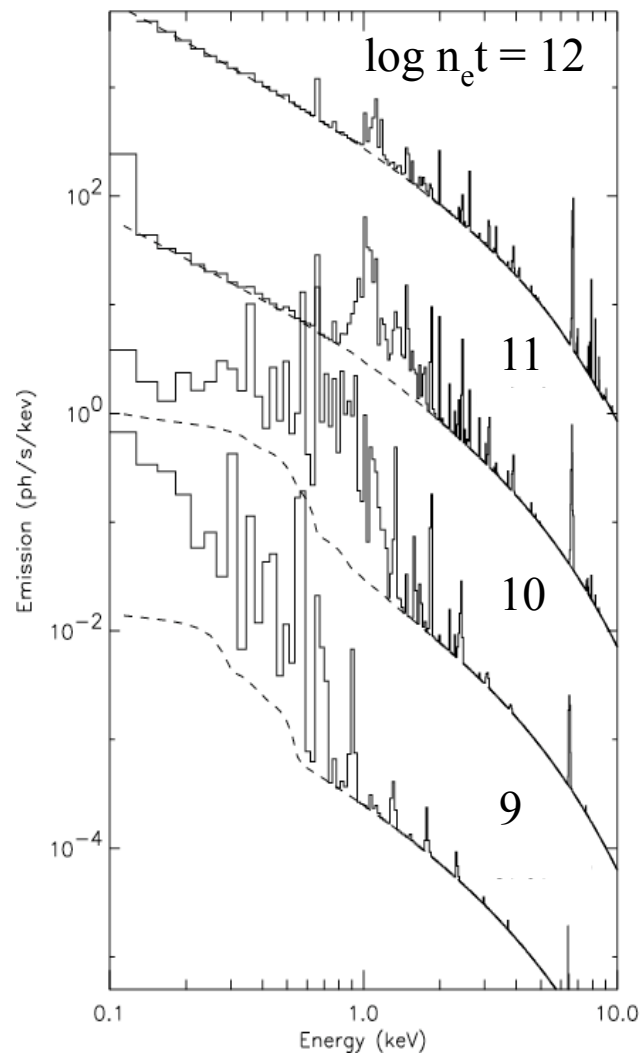
Non-equilibrium ionisation (NEI)

- When gas is suddenly heated (e.g. due to shock) it takes time to ionise it through collisions: the lower n , the longer it takes

$$\frac{1}{n_e(t)} \frac{d}{dt} \vec{n}(Z, t) = \mathbf{A}(Z, T(t)) \vec{n}(Z, t)$$

$$\mathbf{A} = \begin{pmatrix} -I_0 & R_1 & 0 & 0 & \dots & & \\ I_0 & -(I_1 + R_1) & R_2 & 0 & & & \\ 0 & I_1 & \dots & \dots & & & \\ & \vdots & \ddots & \vdots & & & \\ & & & \dots & R_{Z-1} & 0 & \\ & \dots & 0 & I_{Z-2} & -(I_{Z-1} + R_{Z-1}) & R_Z & \\ & & \dots & 0 & I_{Z-1} & -R_Z & \end{pmatrix}.$$

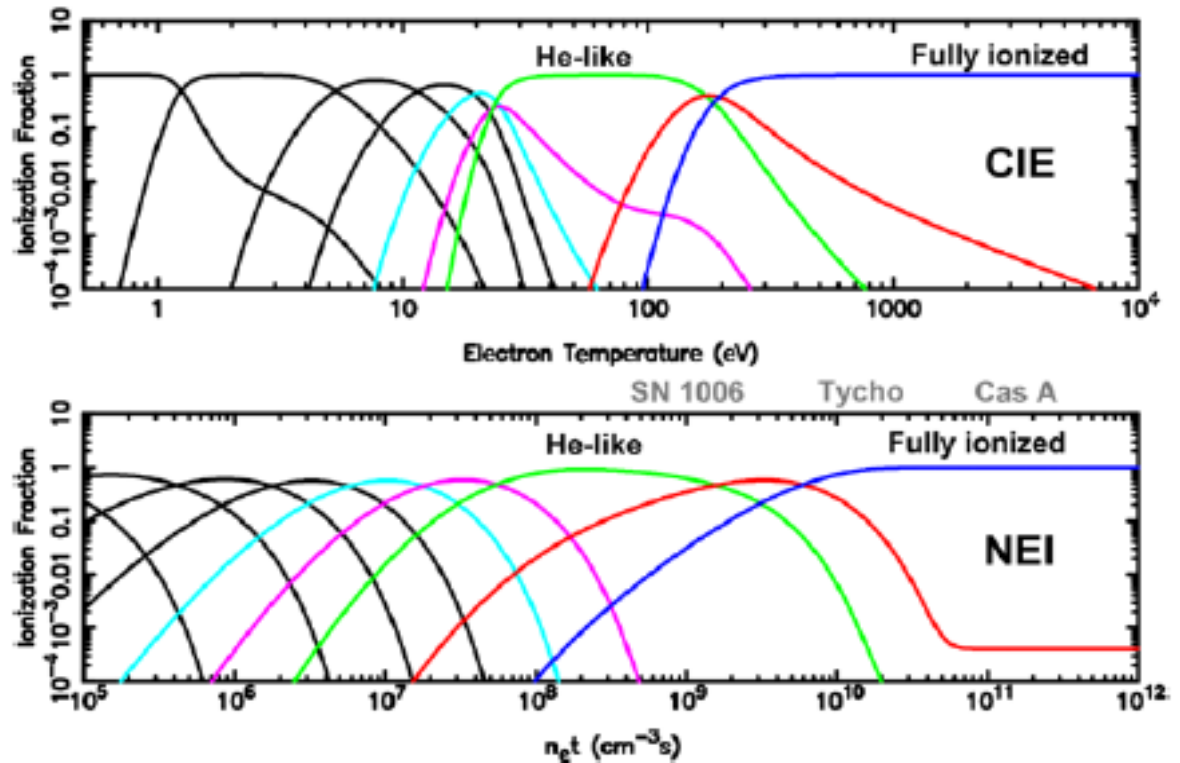
NEI (II)



- Solution depends only on $T(t)$ and the following parameter: $U = \int n_e dt$
- Example supernova remnants: $n_e \sim 1 \text{ cm}^{-3}$, takes $O(1000 \text{ yr})$ to ionise

Comparison CIE/NEI

- CIE ion concentrations oxygen ions
- Compare to NEI for $T=1.5$ keV

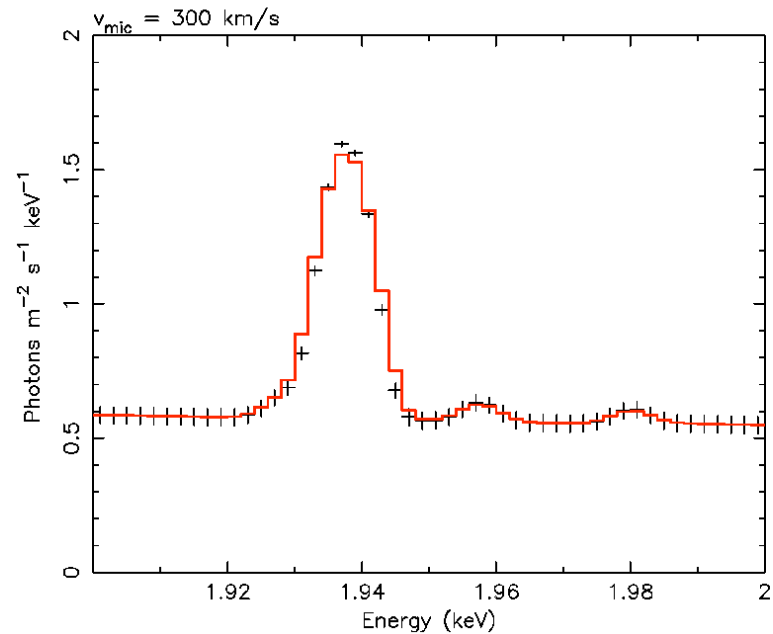


Pictures courtesy Jacco Vink

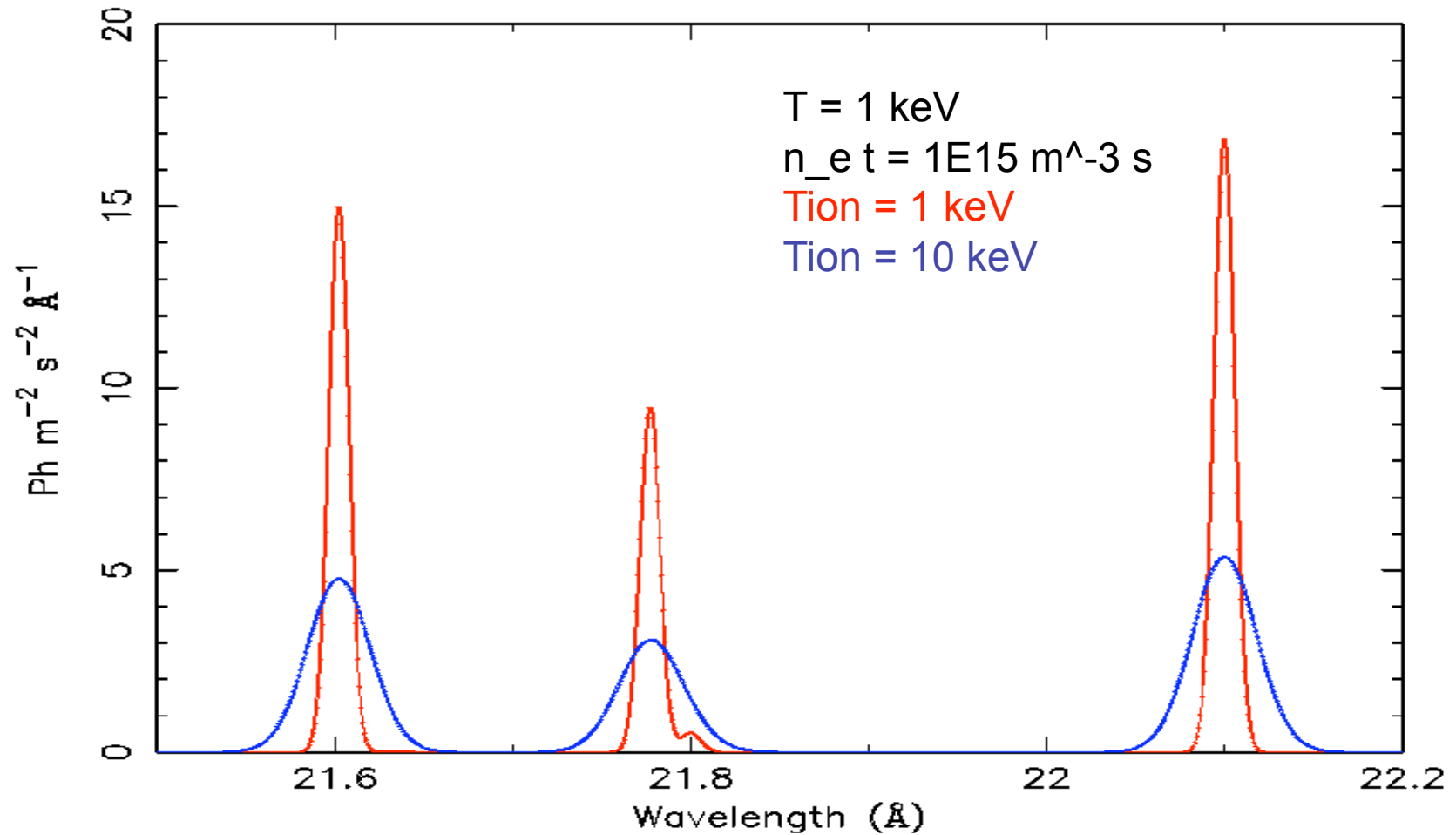
Plasma diagnostics

Turbulence easy to measure...

- Example: 2A0335+096, 100 ks simulation cluster core with Astro-H
- Data: no broadening
- **Model: 300 km/s**
- Example here for Si XIV, much better of course for Fe
- **But: need to pay attention to calibration!**

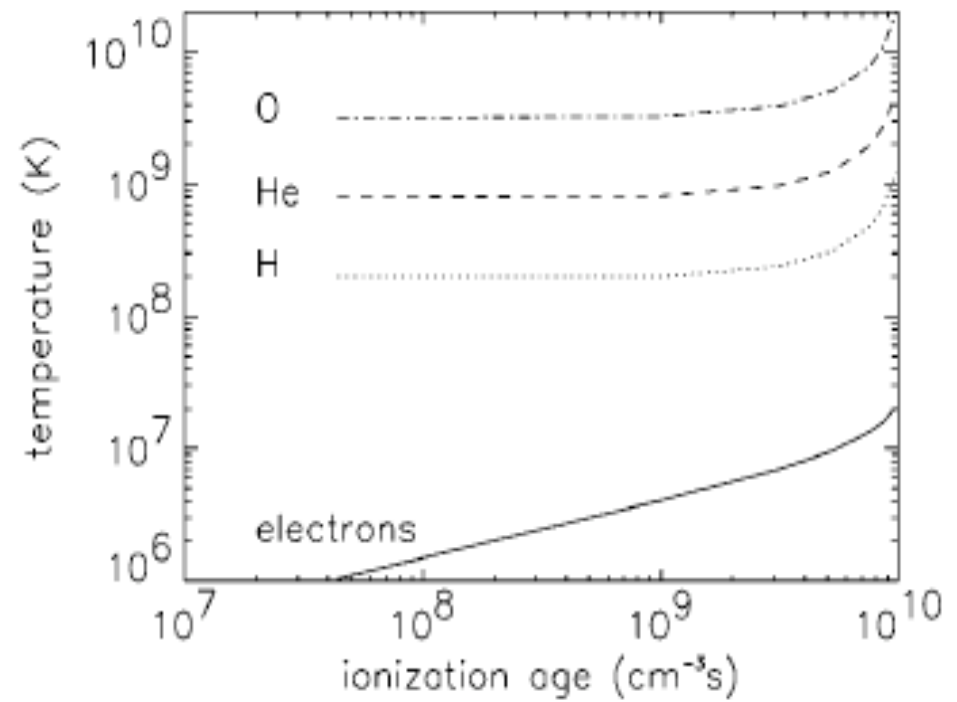
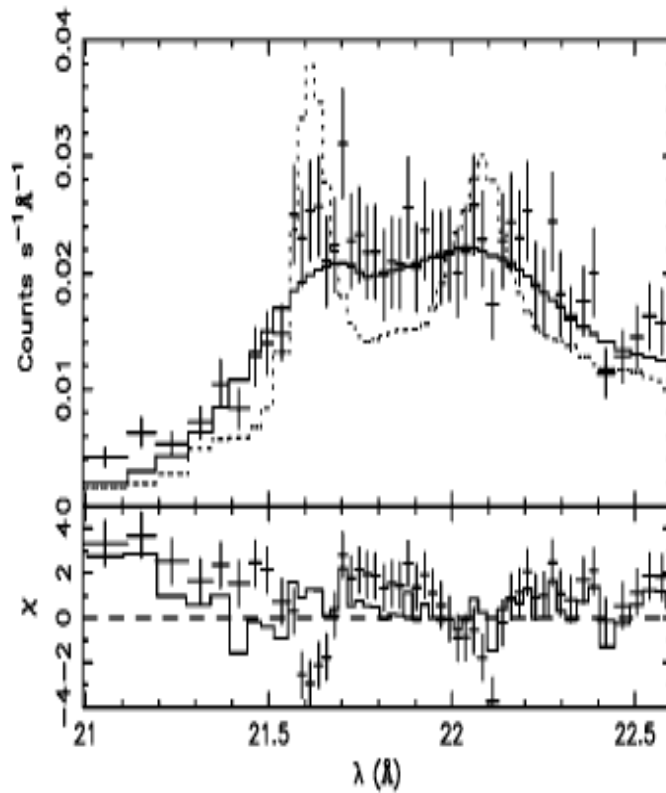


Ion temperatures

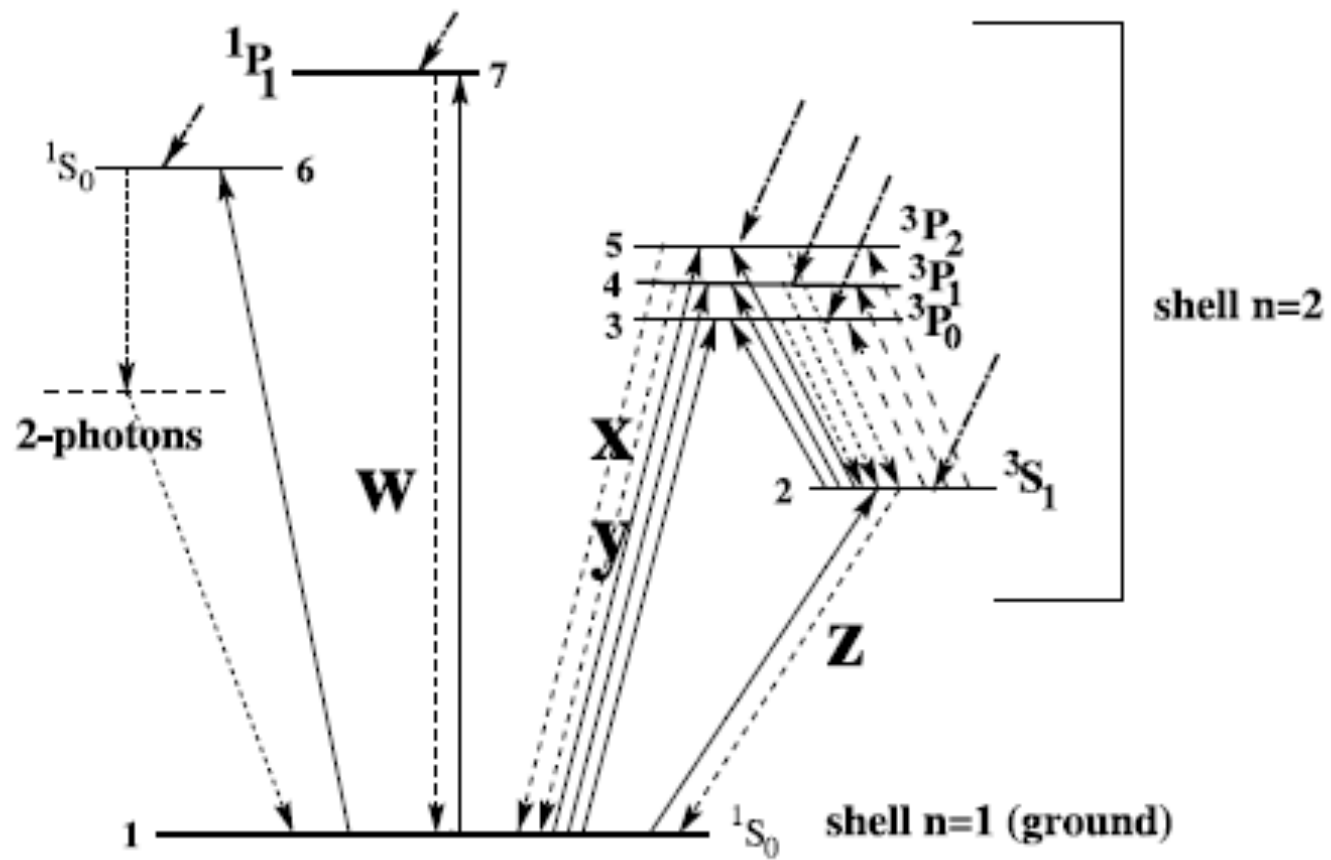


Non-equilibrium: measuring ion temperatures

(Vink et al. 2003)

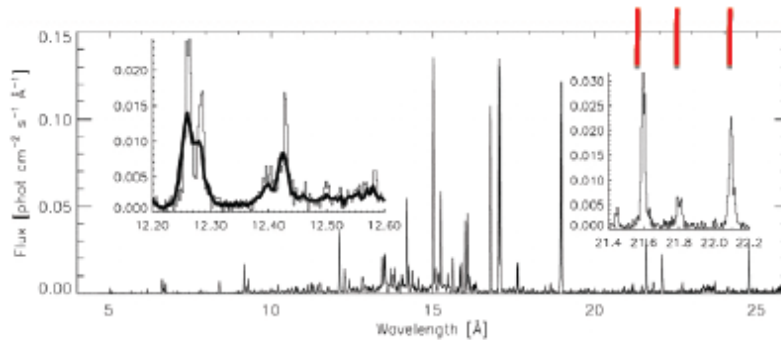


He-like ions

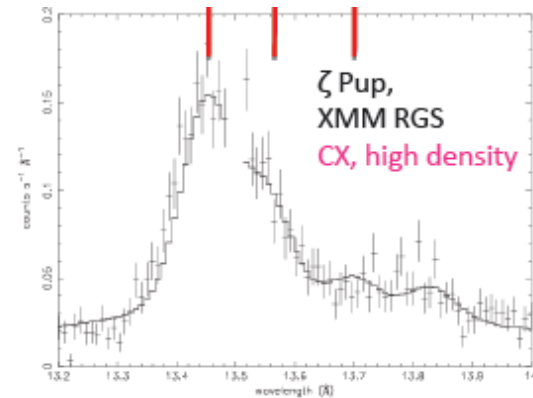


Examples of He-like triplets

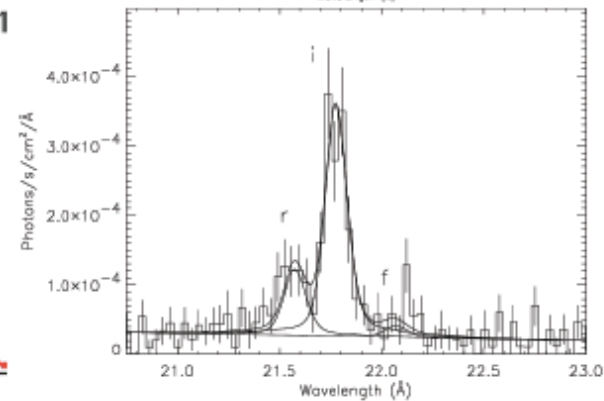
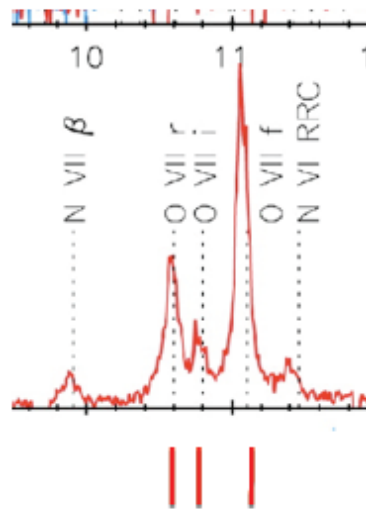
(picture courtesy Frits Paerels)



Capella, *Chandra* HETGS:
CX, low density



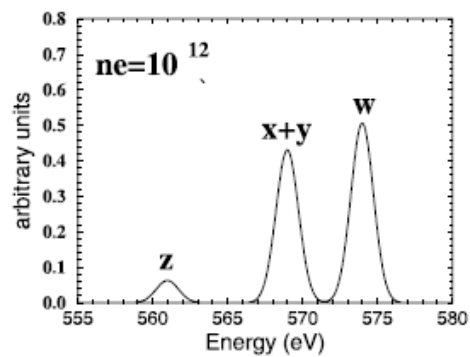
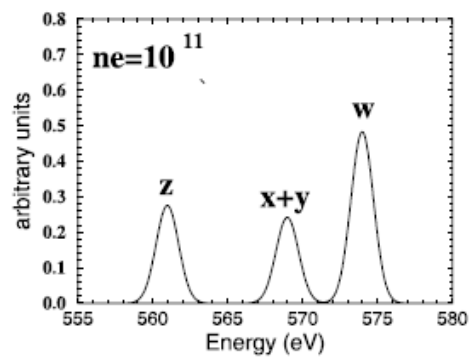
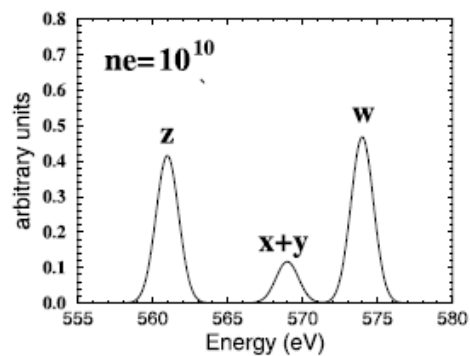
NGC 1068, RGS
XP, low density



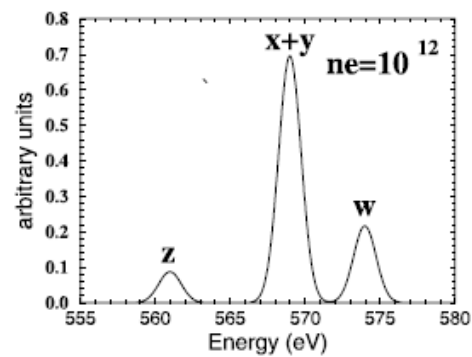
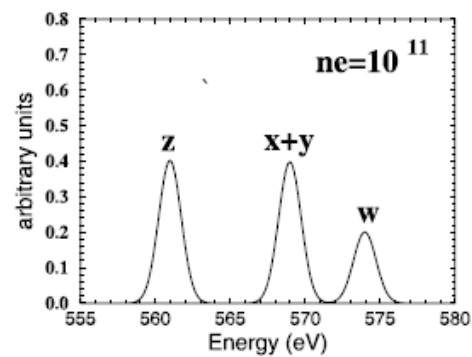
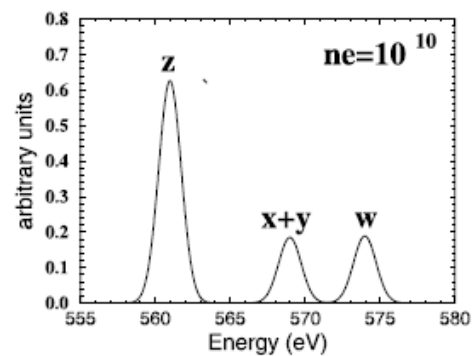
EXO0748-676, RGS
XP, high density

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

Collisional ionisation



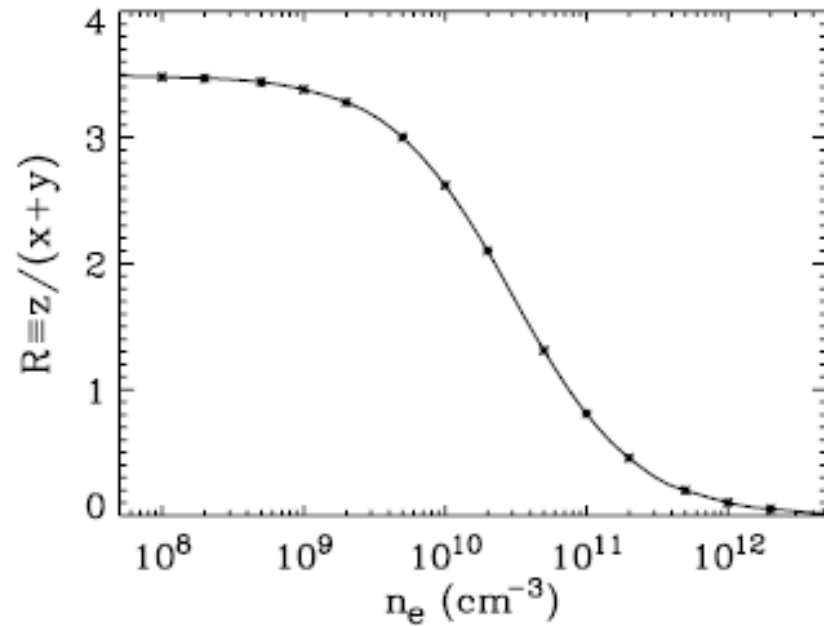
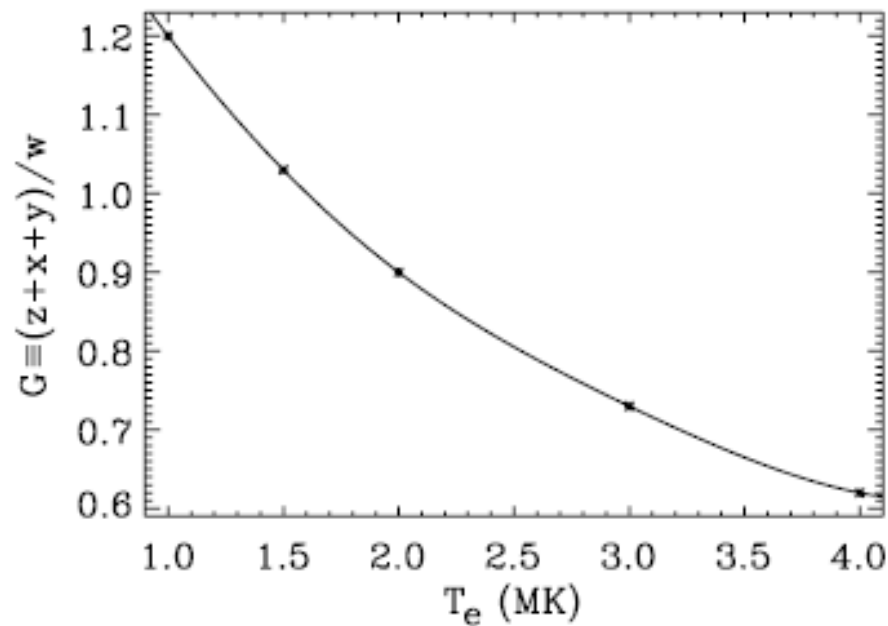
Photoionisation



See Porquet
2011

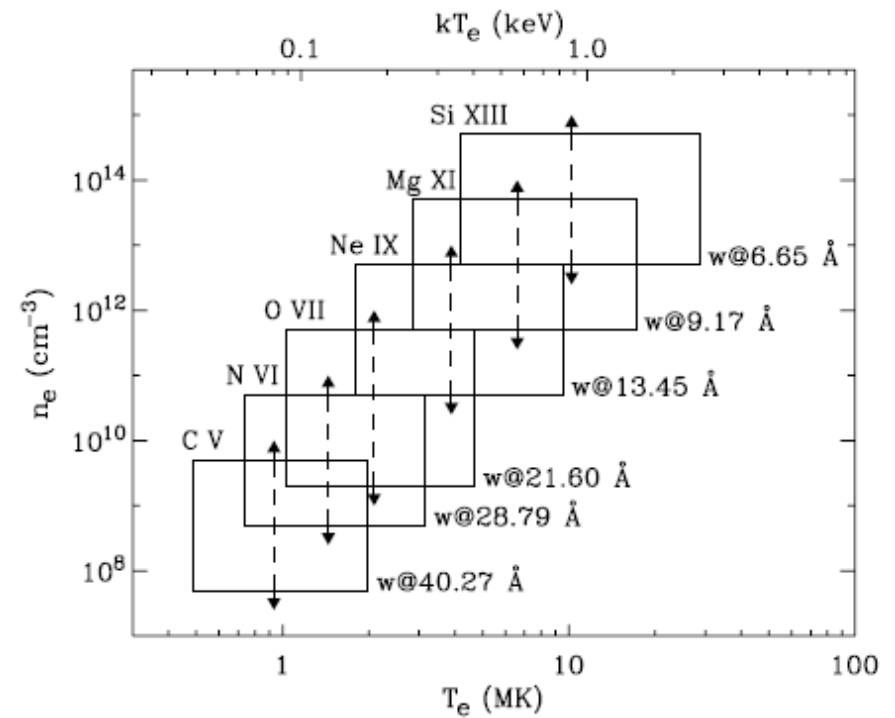
Example: O VII

(Porquet et al. 2001)



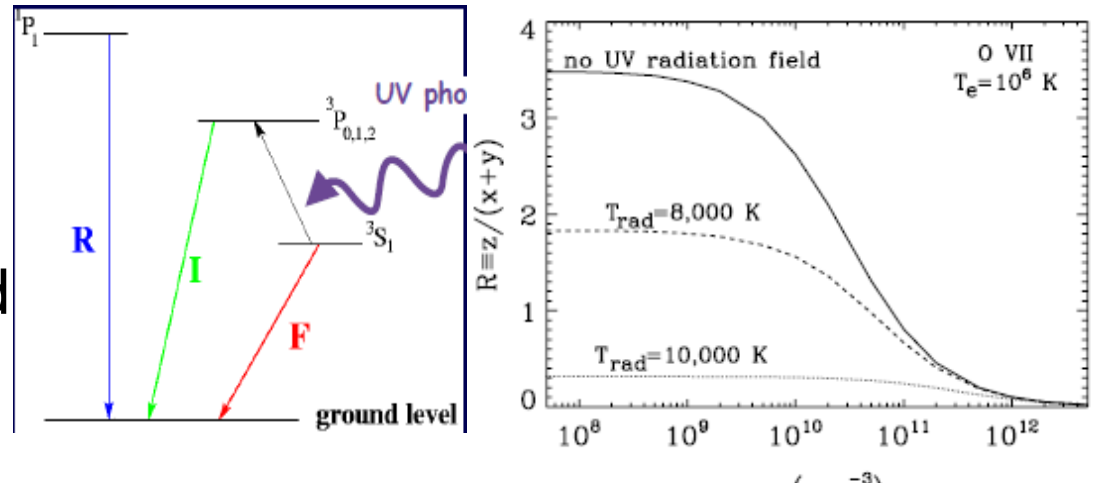
Density diagnostics triplets

(Porquet et al. 2011)

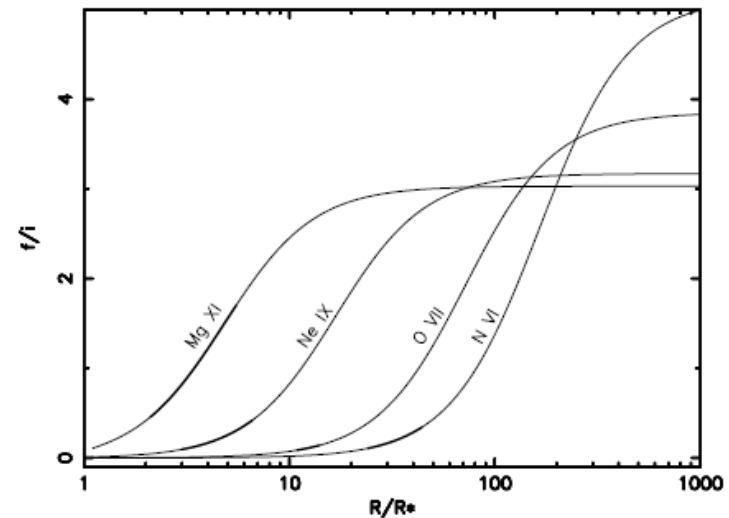


Dependence on UV radiation field

- Forbidden & intercombination upper level coupled also by radiation field
- Strong UV field → altered ratio; can mimic high density!
- Example: star ζ Ori, $T=30000$ K

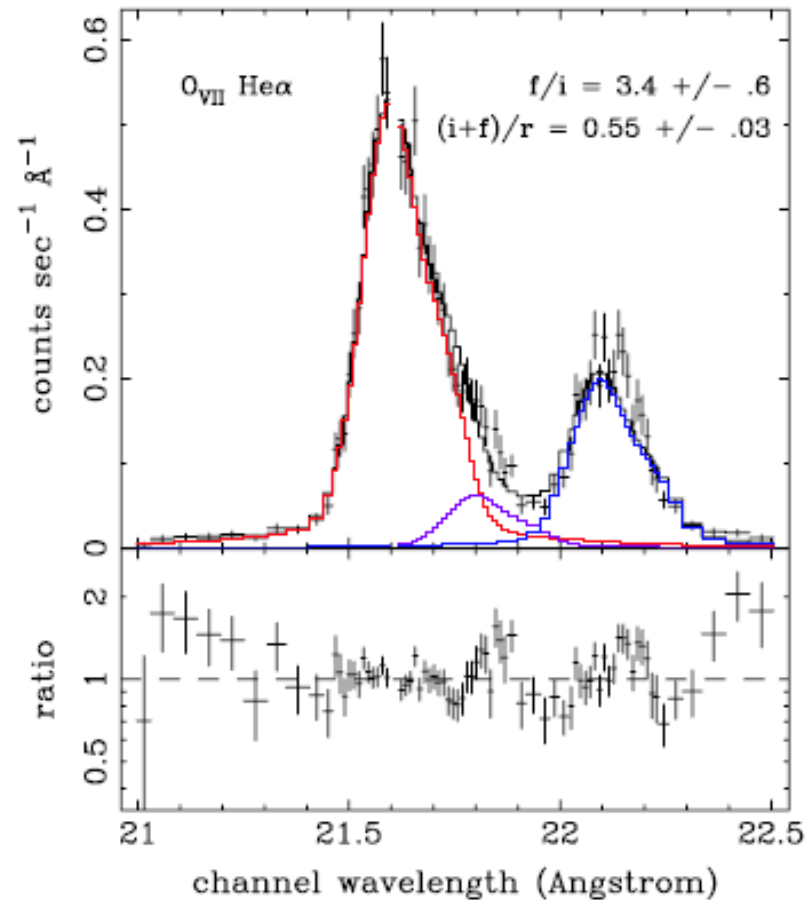


(fig. from Raassen et al. 2008)



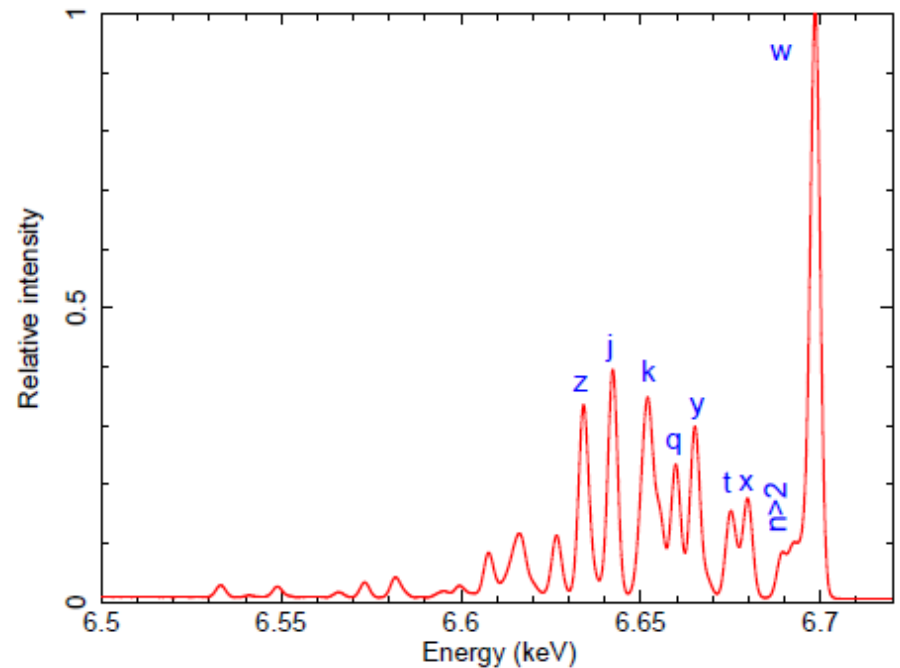
Triplet in NEI plasma

- Ionising plasma has stage with few H-like ions \rightarrow few recombinations onto He-like \rightarrow weaker f+i line \rightarrow lower $G=(i+f)/r$ ratio compared to CIE case
- Example: 1E0102 supernova remnant (Rasmussen et al. 2001)



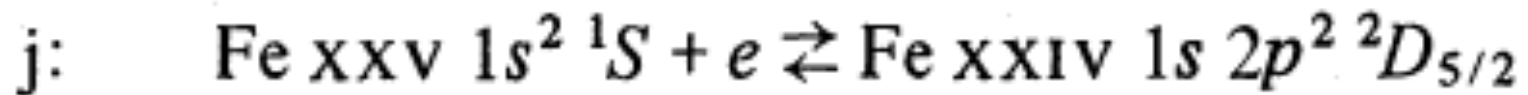
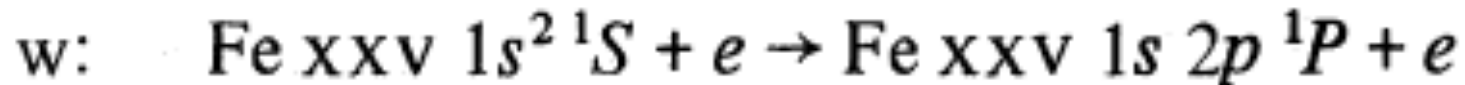
Dielectronic satellite lines

- Example: spectrum in CIE
- $kT = 2$ keV
- Fe XXV He-like triplet: z (forbidden), x&y (intercombination), w (resonance)
- Most other labelled lines Fe XXIV satellite lines
- Lines @ $E < z$ -line Fe XXIII
- Some sensitive to non-thermal electrons



Non-thermal electrons

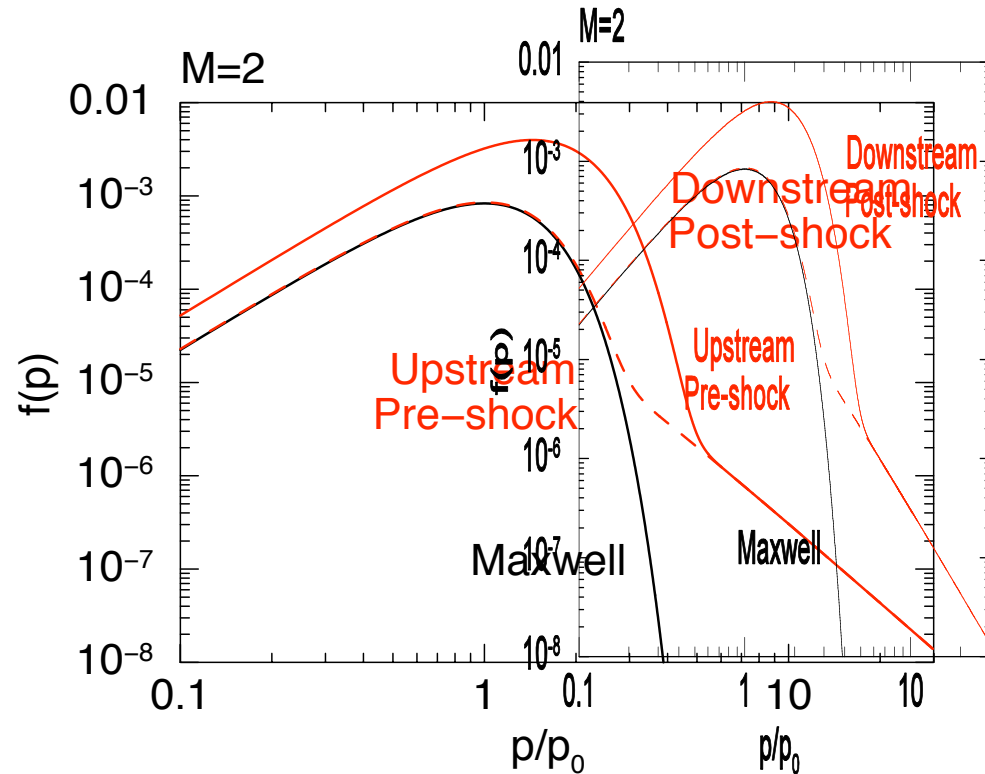
(Gabriel & Phillips 1979)



- j-line only excited by free electrons of $E=4.694$ keV (capture free electron & excite one 1s electron)
- w-line sensitive to all electrons Maxwellian & above (suprathermal electrons)
- **→** j/w line ratio lower when suprathermal electrons are present

Detecting non-thermal electrons

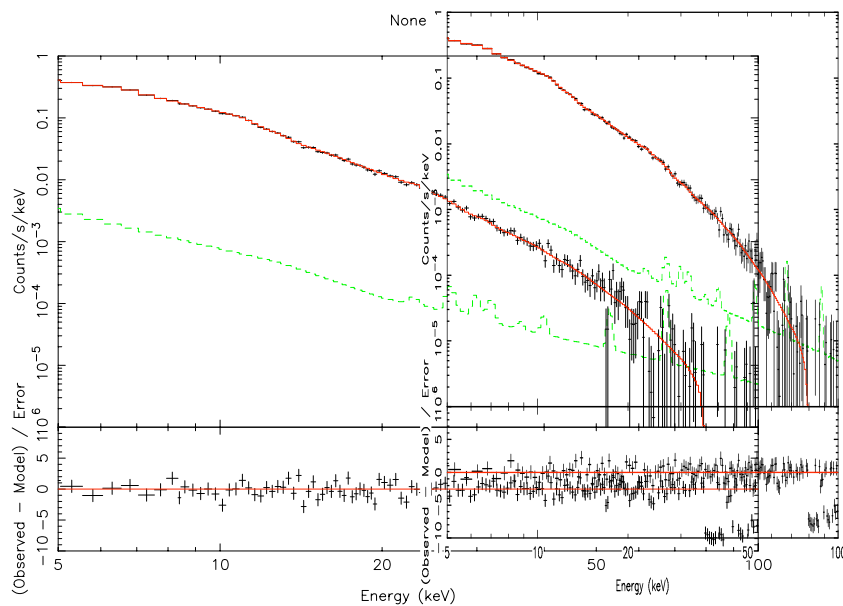
- Particle acceleration in many sources (shocks, flares, etc)
- How to detect non-thermal tails?



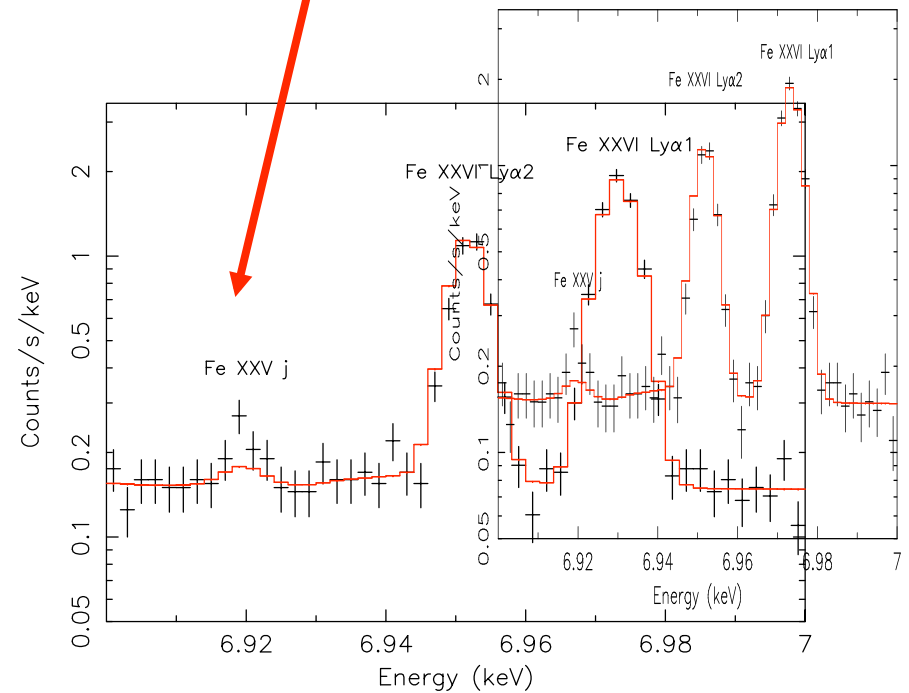
shock in hot cluster (Kaastra, Bykov & Werner 2009)

Astro-H HXI and SXS

Fit with thermal plasma only
already acceptable



Satellite lines provide the
answer!



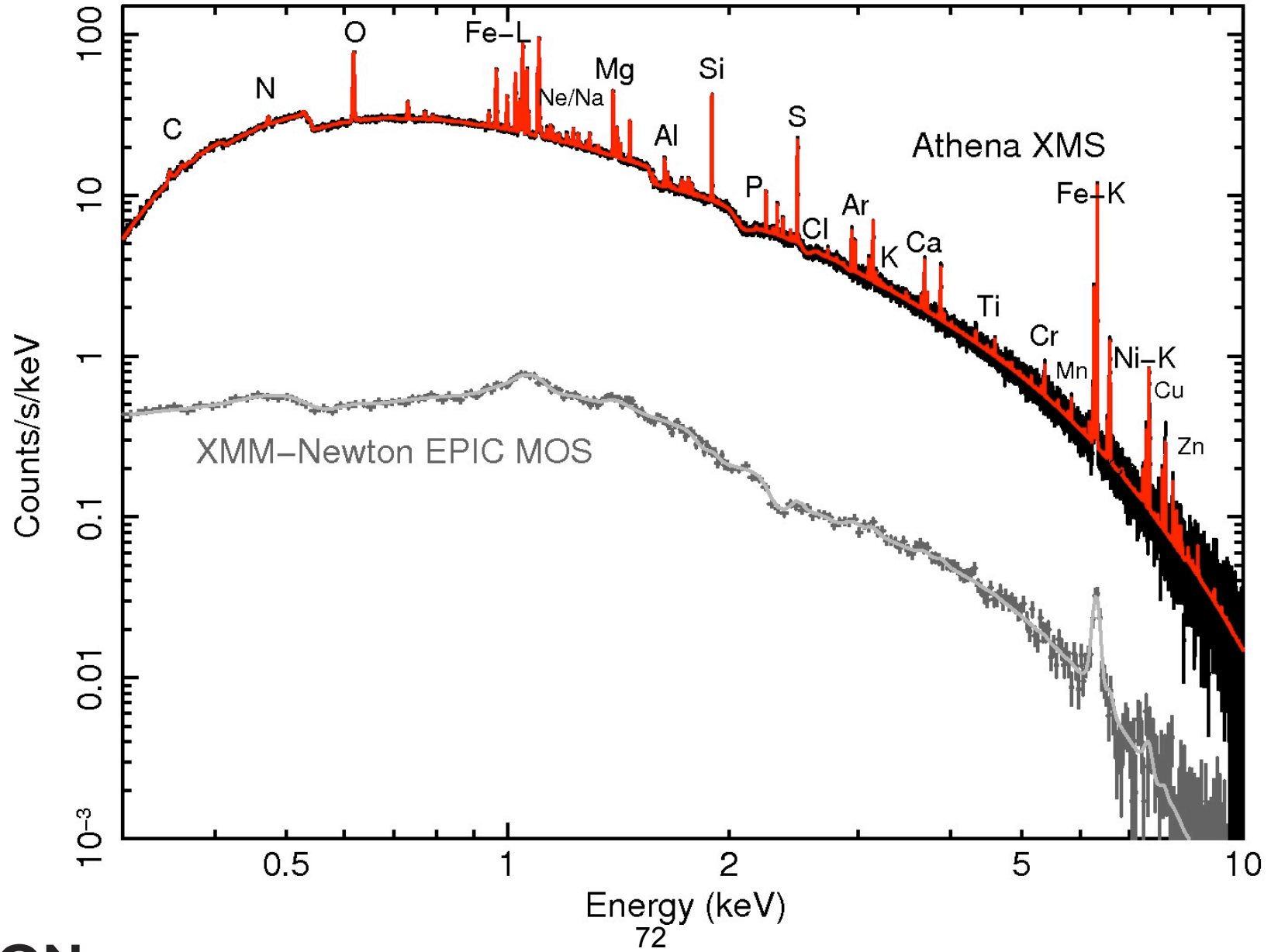
Abundances

- *Absorption studies*: line properties do not depend strongly on Z → most abundant metals (O) most prominent
- *Emission studies*: emissivity strong function of Z → bias towards high- Z (Fe) lines prominent

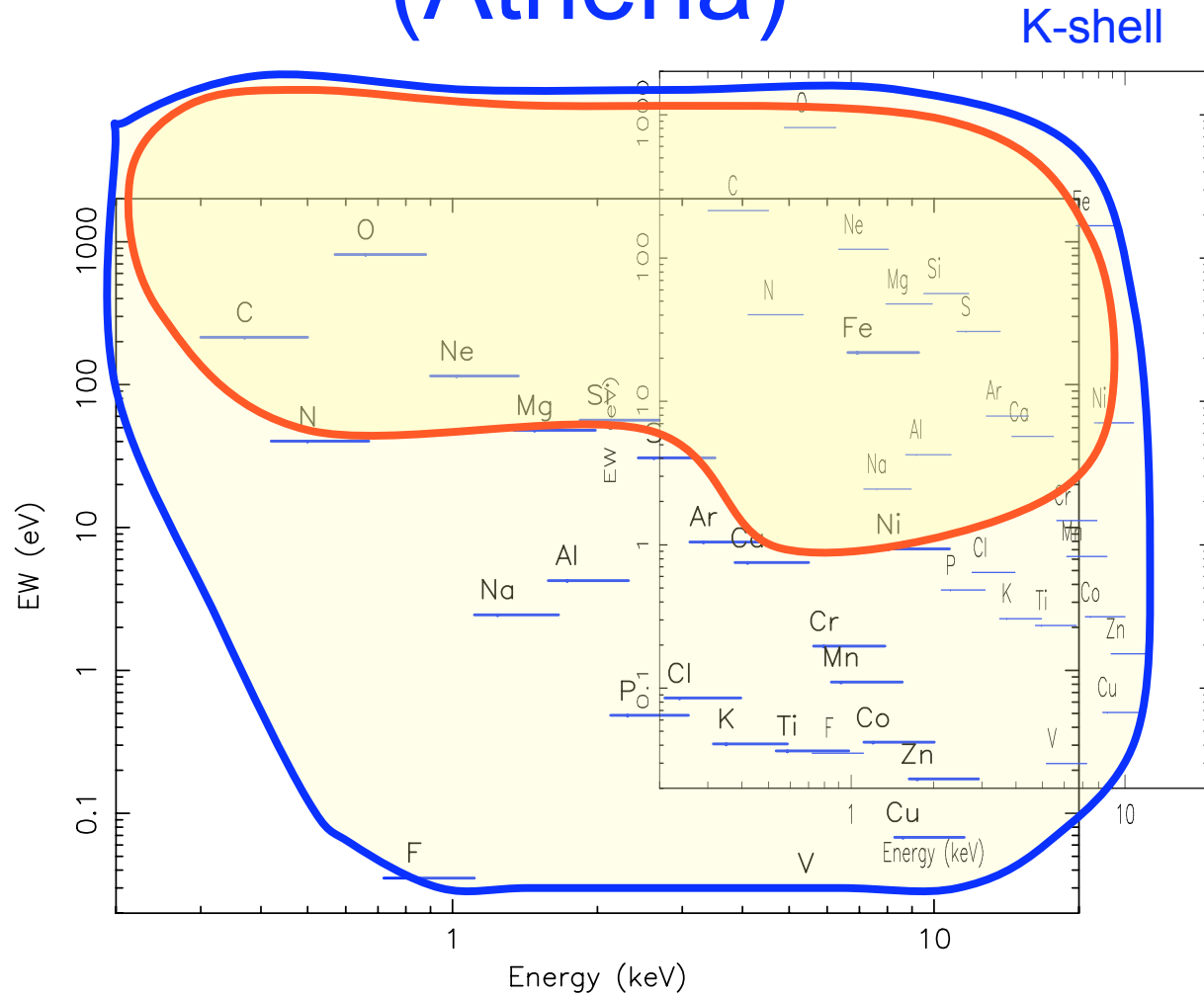
Table 3.4: Proto-Solar abundances for the 15 most common chemical elements. Abundances A are given with respect to hydrogen. Data from Lodders (2003).

Element	abundance	Element	abundance	Element	abundance
H	$\equiv 1$	Ne	89.1×10^{-6}	S	18.2×10^{-6}
He	0.0954	Na	2.34×10^{-6}	Ar	4.17×10^{-6}
C	288×10^{-6}	Mg	41.7×10^{-6}	Ca	2.57×10^{-6}
N	79.4×10^{-6}	Al	3.47×10^{-6}	Fe	34.7×10^{-6}
O	575×10^{-6}	Si	40.7×10^{-6}	Ni	1.95×10^{-6}

Abell 1795 (100 ks)



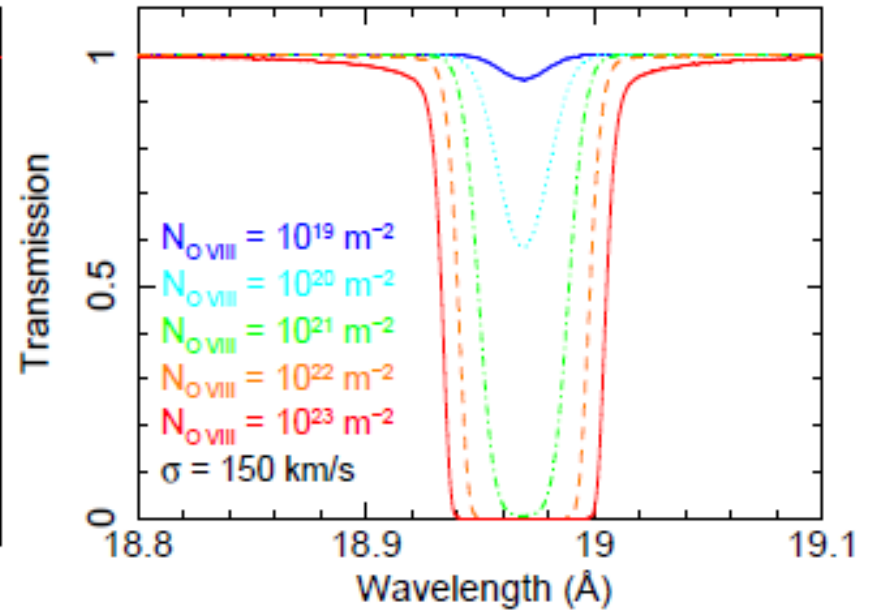
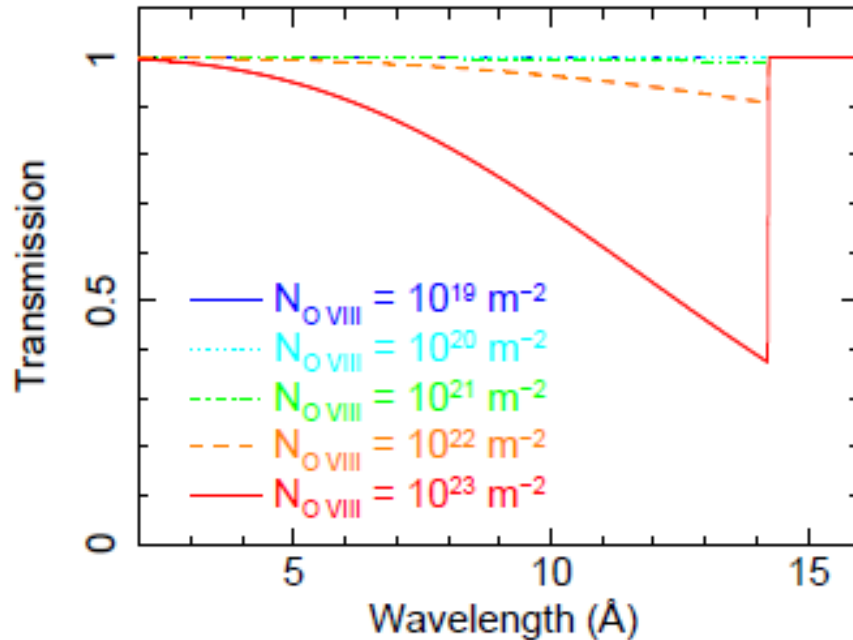
Which elements will we see? (Athena)



Absorption spectra

Continuum versus line absorption

Example: O VIII



Continuum absorption

$$\tau_{\text{cont}}(E) \equiv N_{\text{H}}\sigma_{\text{cont}}(E) = \sum_i N_i\sigma_i(E)$$

$$T(E) = \exp(-\tau_{\text{cont}}(E))$$

Line absorption

The transmission in a spectral line at wavelength λ is given by

$$T(\lambda) = e^{-\tau(\lambda)}$$

with

$$\tau(\lambda) = \tau_0 \varphi(\lambda)$$

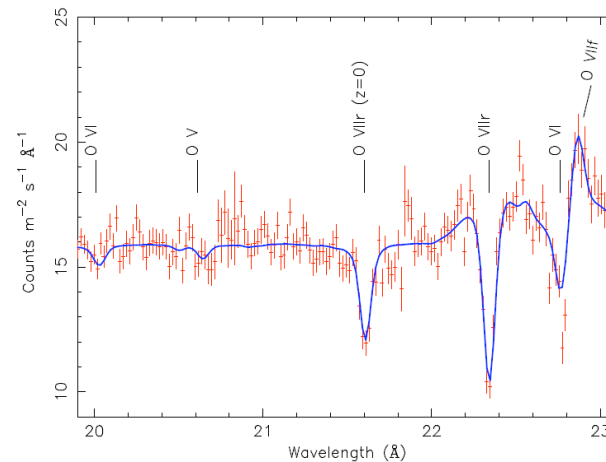
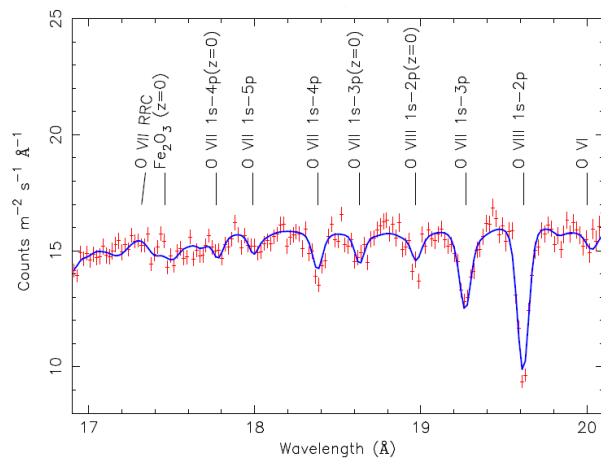
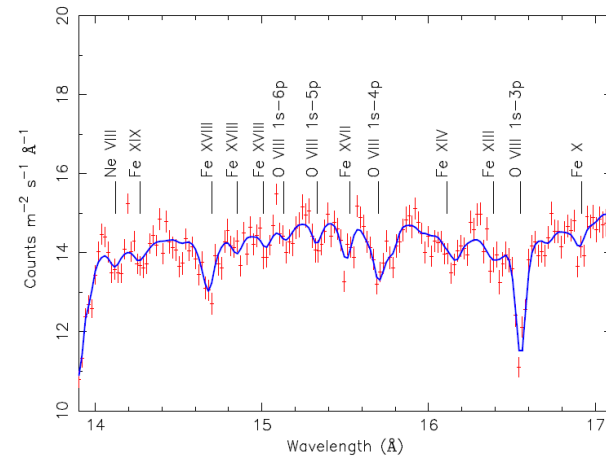
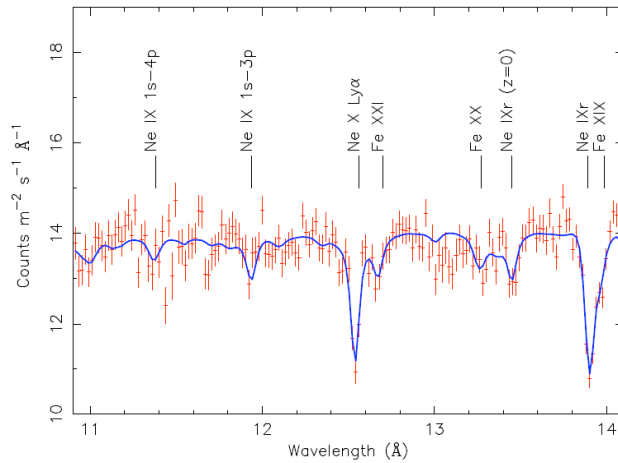
where $\varphi(\lambda)$ is the line profile and τ_0 is the opacity at the line centre λ_0 , given by:

$$\tau_0 = \frac{\alpha h \lambda f N_i}{2\sqrt{2\pi} m_e \sigma_v}$$

Apart from the fine structure constant α and Planck's constant h , the optical depth also depends on the properties of the absorber, namely the ionic column density N_i and the velocity dispersion σ_v . Furthermore, it depends on the oscillator strength f which is a dimensionless quantity that is different for each transition and is of order unity for the strongest transitions.

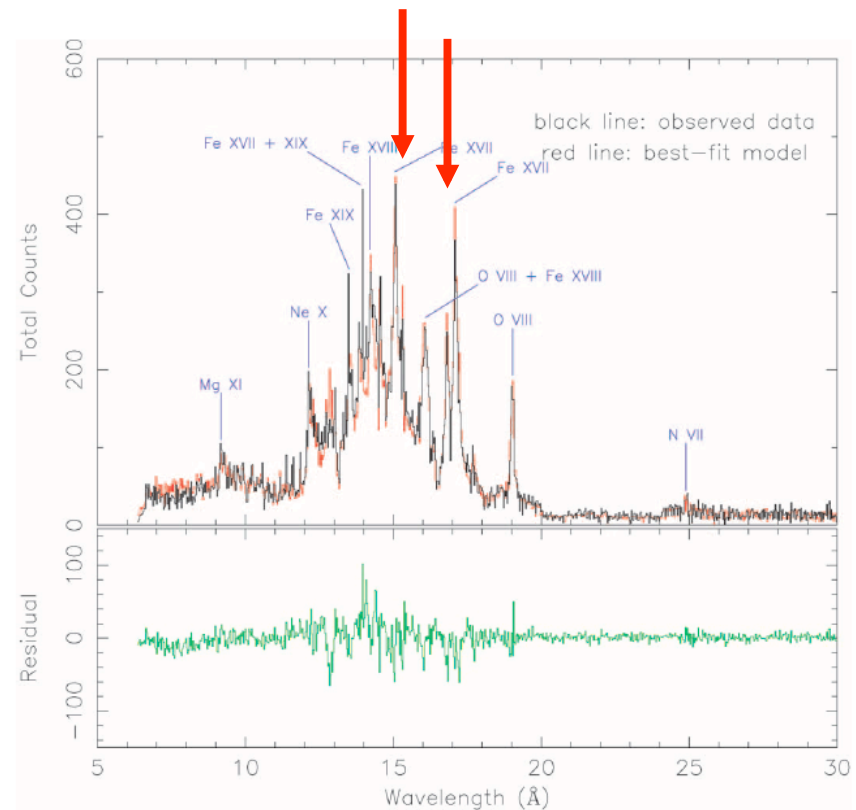
Sample high-resolution absorption spectra

(Mrk 509, Seyfert galaxy, 600 ks RGS data; Detmers et al. 2011)



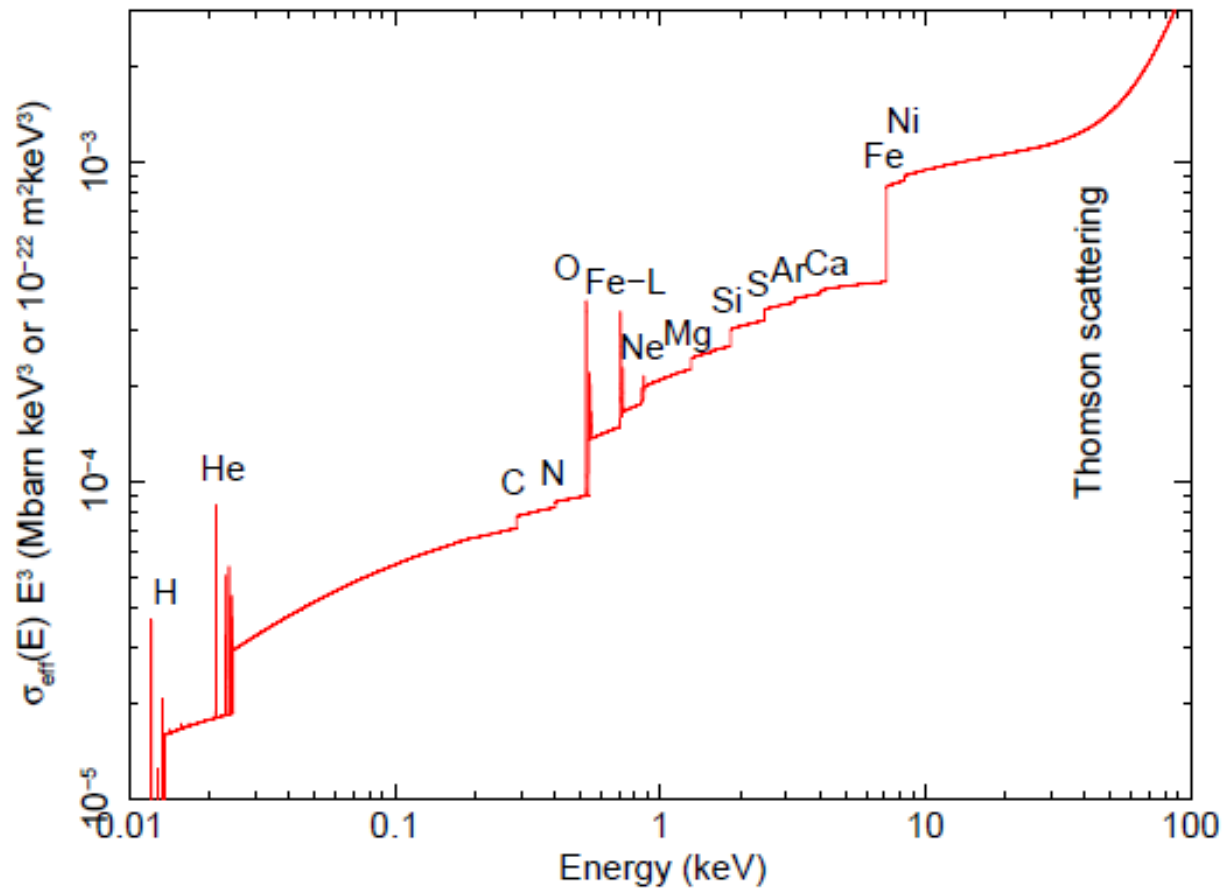
Resonance scattering

- Alternative to measure turbulence
- Fe XVII 15.02 to 17.05/17.10 ratio sensitive to res. scat. (τ depends on turbulence)
- Currently only RGS can do it (see also Werner et al. 2009)
- SXS can map it

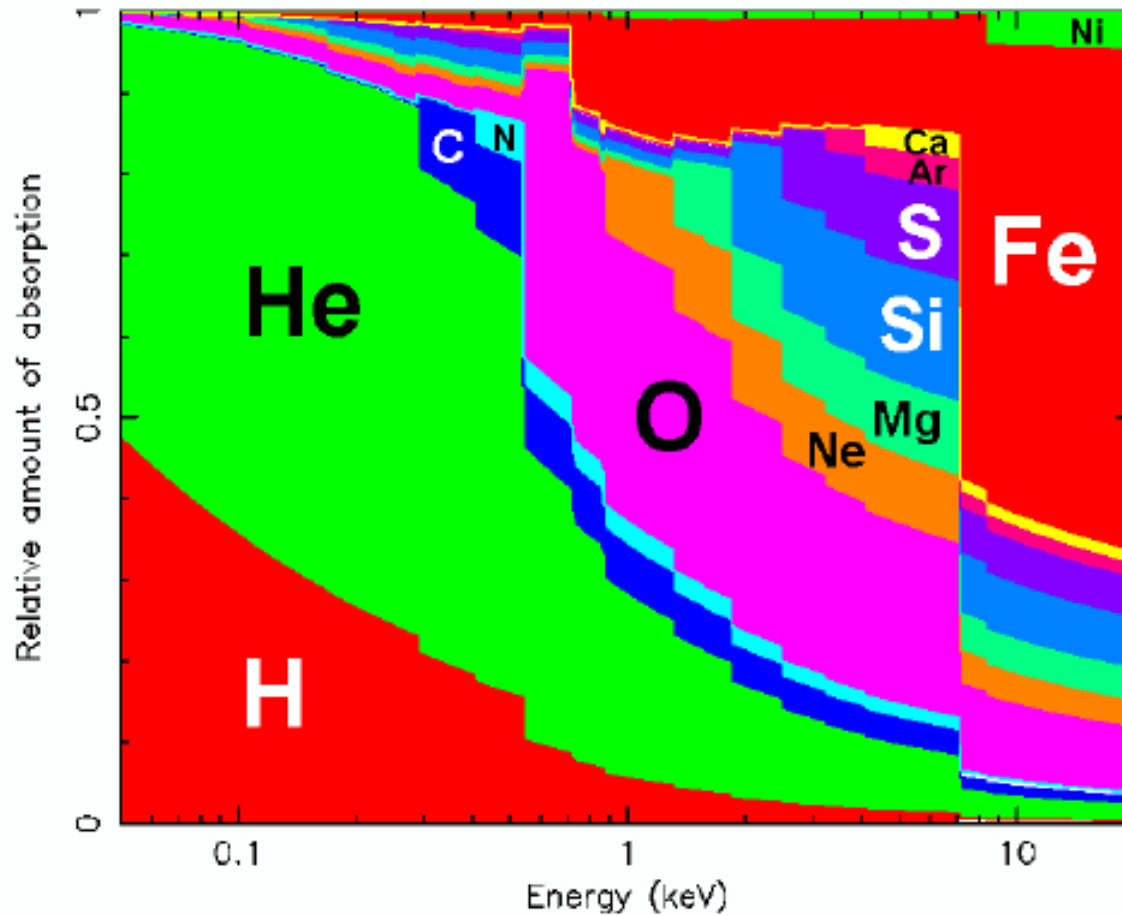


Xu et al. 2002, NGC 4636

Example: Interstellar medium opacity



Contribution of the elements to the ISM opacity



Dust depletion

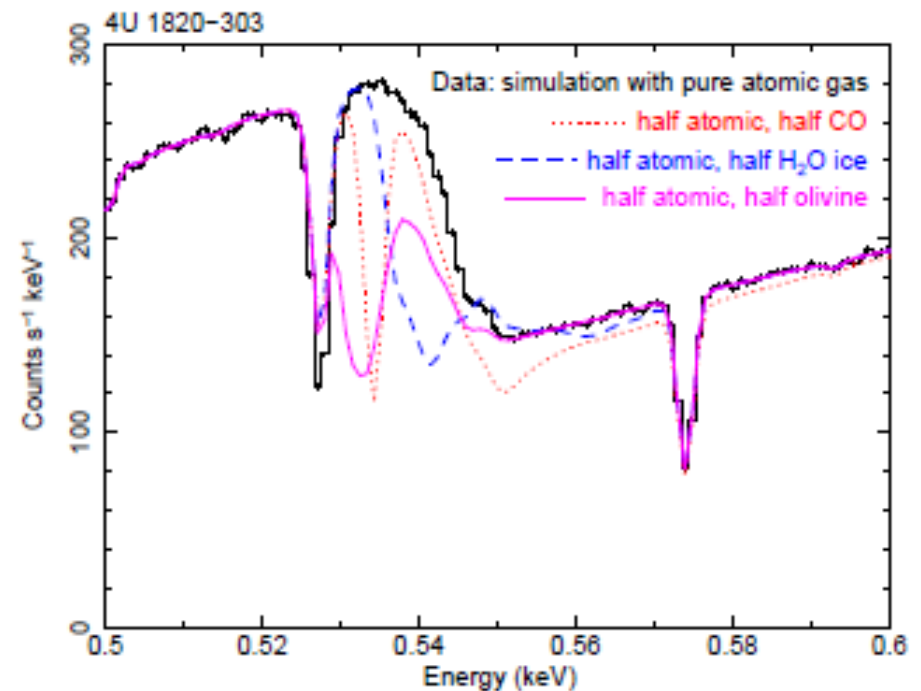
Another ISM component is **dust**. A significant fraction of some atoms can be bound in dust grains with varying sizes, as shown below (from Wilms et al. 2000):

H	He	C	N	O	Ne	Mg	Si	S	Ar	Ca	Fe	Ni
0	0	0.5	0	0.4	0	0.8	0.9	0.4	0	0.997	0.7	0.96

The numbers represent the fraction of the atoms that are bound in dust grains. Noble gases like Ne and Ar are chemically inert hence are generally not bound in dust grains, but other elements like Ca exist predominantly in dust grains.

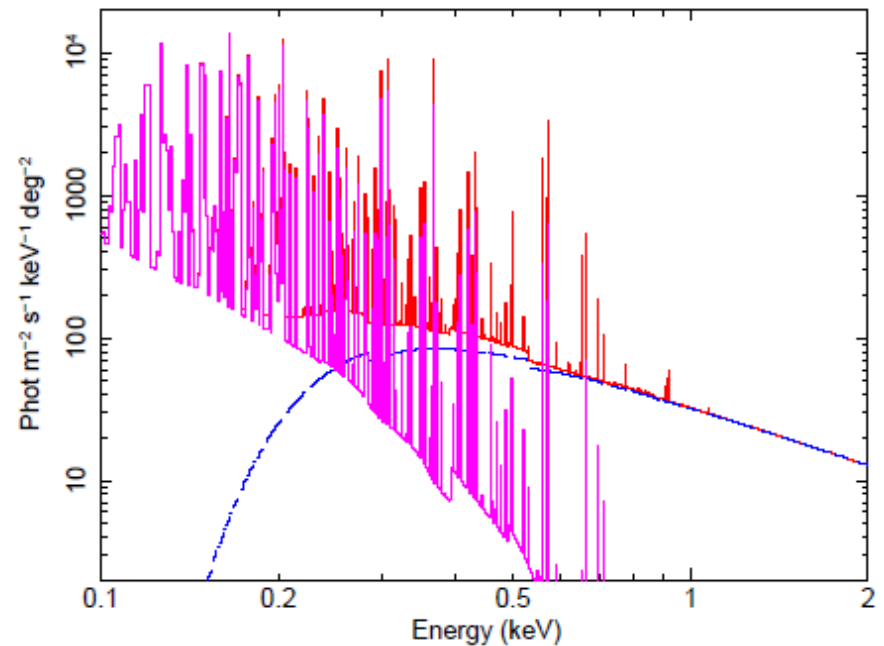
Spectral signatures of dust

- Atomic structure changes when atom bound in molecule
- Example: H_2O
- Study of fine structure near edges \rightarrow chemical structure
- Uncertainties/lacking lab data



Galactic foreground emission

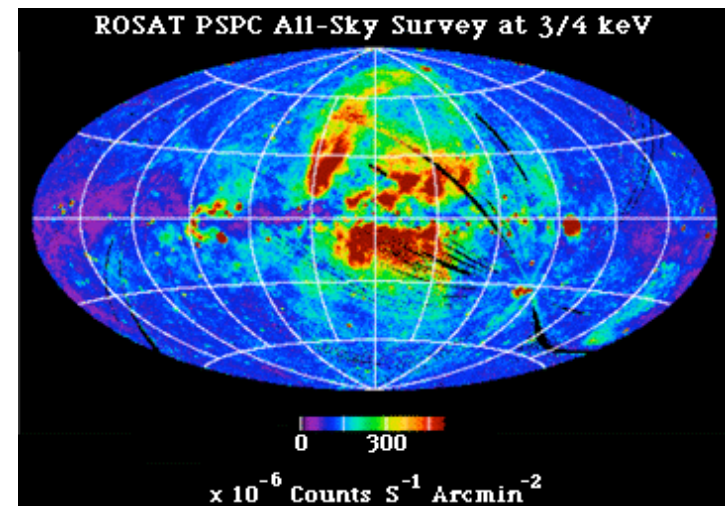
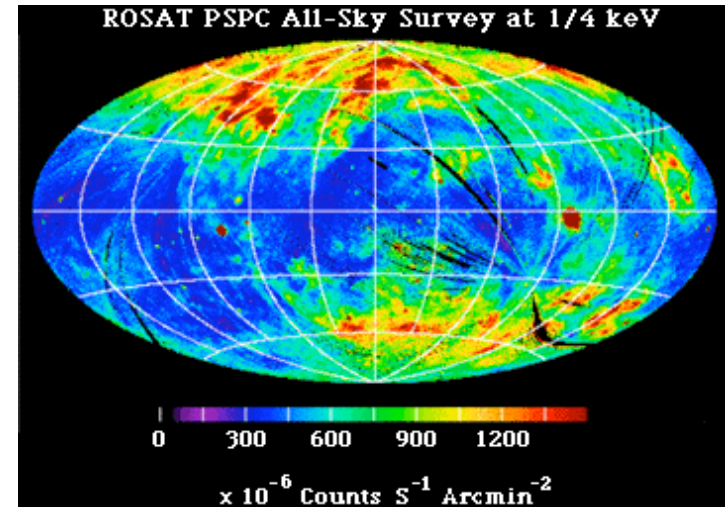
- Emission from more components:
 - Local Hot Bubble (kT=0.1 keV)
 - Distant local components (kT=0.2 keV)
 - Extragalactic power law (unresolved point sources)
 - Solar wind charge exchange emission: time variable



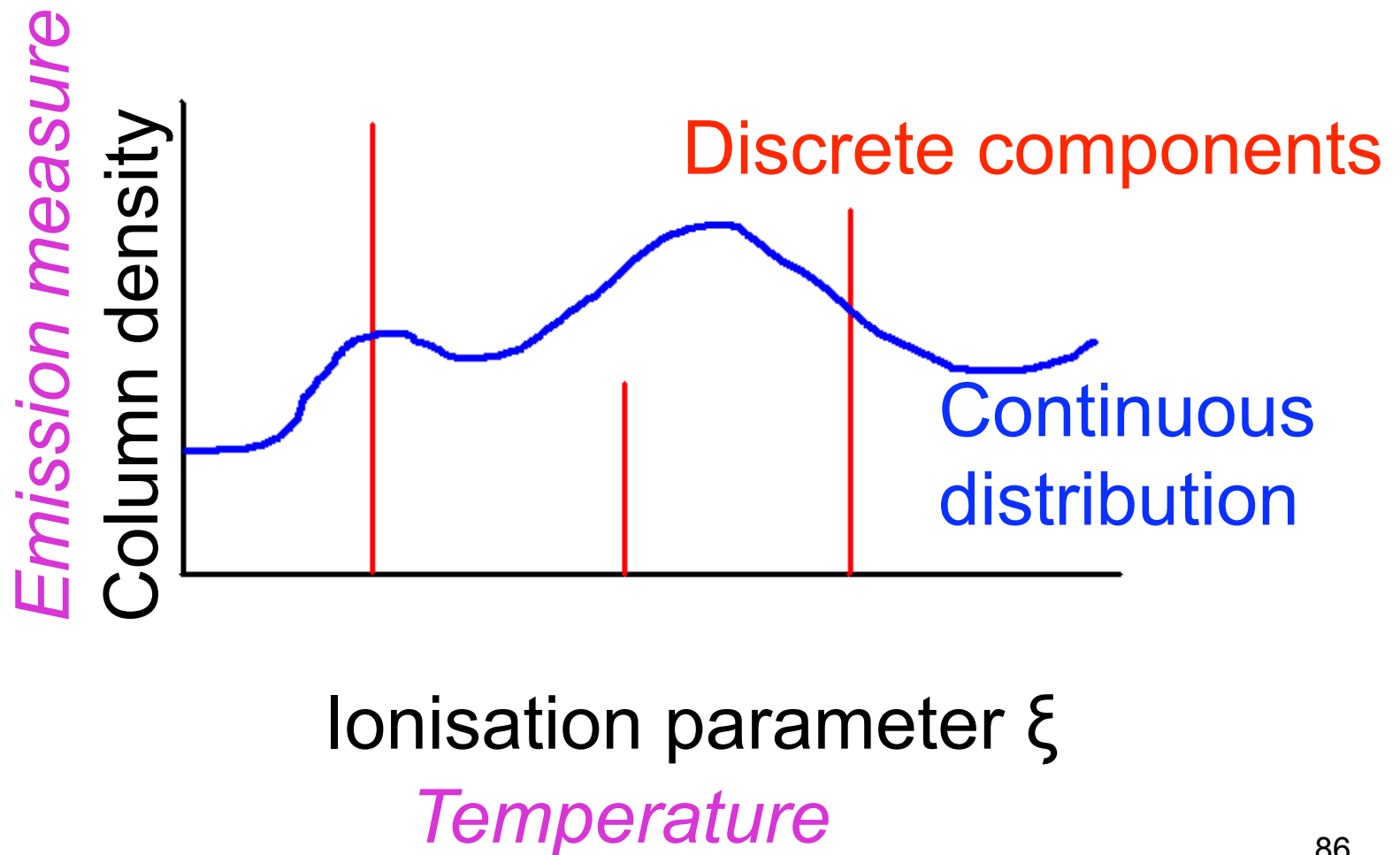
ISM is not homogeneous

Many components:

- Hot ionised 10^6 K
- Warm ionised 8000 K
- Warm atomic
6000-10000 K
- Cold atomic 20-50 K
- Molecular 10-20 K
- dust



Absorption measure distribution



Spectroscopic consistency versus formal detection significance

- Think you see a line:
- Check if other instrument sees same line (example: Buote et al. 2009, Sculptor wall)
- Are there other lines from the same ion? Example: Mrk 509 O VIII lines

