X-RAY SPECTROSCOPY in ASTROPHYSICS

General literature

1. P. McWhirter: in "Plasma Diagnostic Techniques," Huddlestone & Leonard (Eds.), 1965
2. SM Kahn & DA Liedahl: in "Physics with Multiply Charged Ions", Liesen, D. (Ed.), Plenum Press (1995) [simple intro]
3. R. Mewe: "Atomic Physics of Hot Plasmas" in: 'X-ray Spectroscopy in Astrophysics', J. van Paradijs, J. Bleeker (Eds.), Springer, 1998 [collisional plasmas]
4. D.A. Liedahl: "Spectral Properties of PIE and NIE Plasmas", in: "X-ray Spectroscopy in Astrophysics", J. van Paradijs, J. Bleeker (Eds.), Springer 1998 [radiation dominated & transient plasmas]
5. S.M. Kahn: Lectures at recent Saas-Fee school (not yet, or unpublished)

Preliminaries:

TREMENDOUS progress since launch of Chandra & XMM!

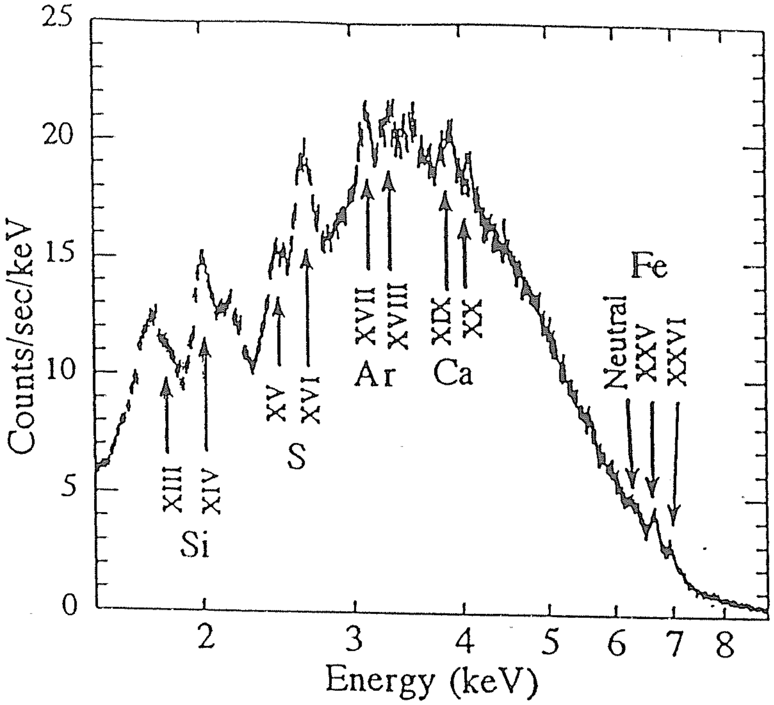
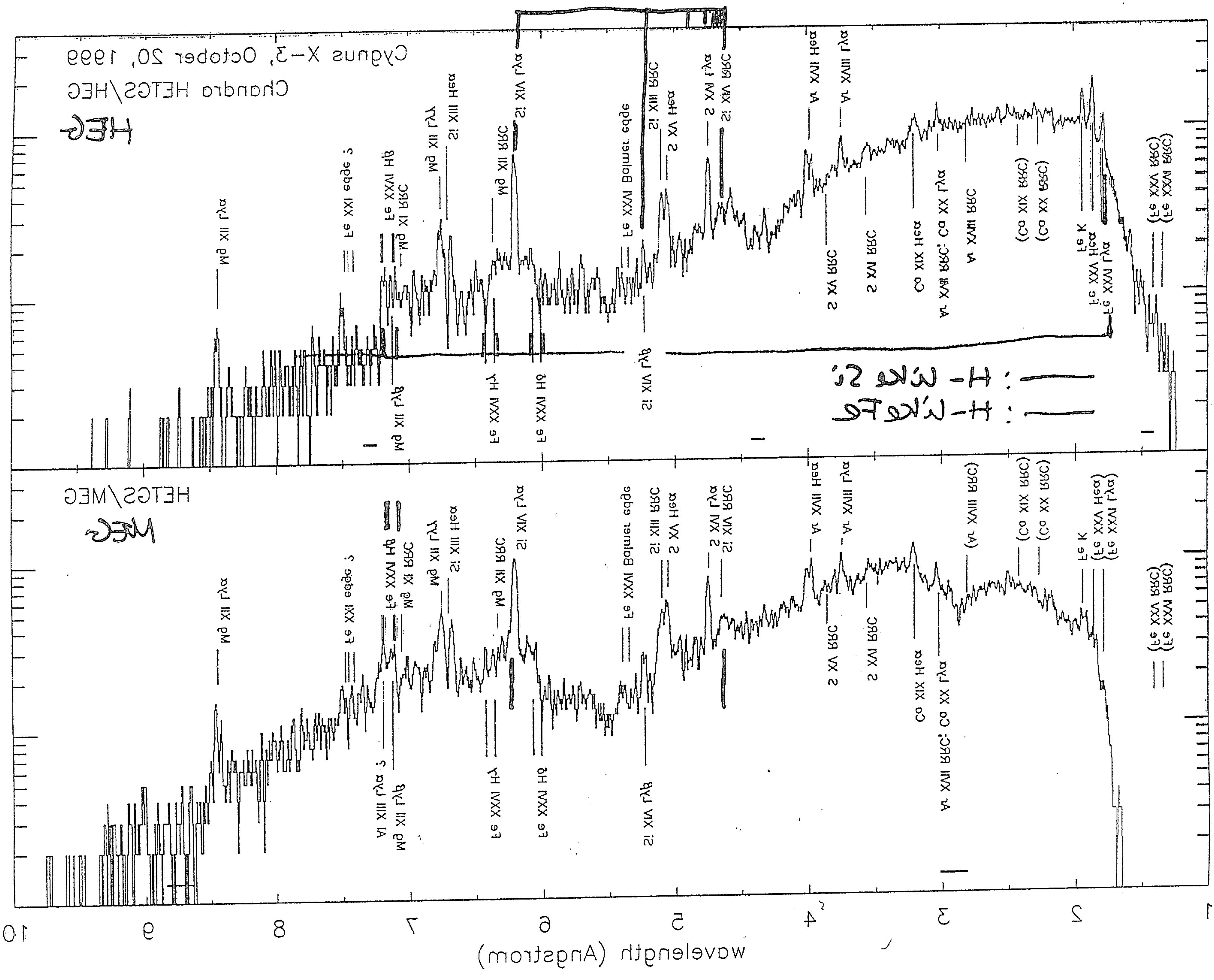


Fig. 1. Energy spectrum of Cyg X-3 obtained by SIS. Identifications for prominent lines are also indicated by arrows.

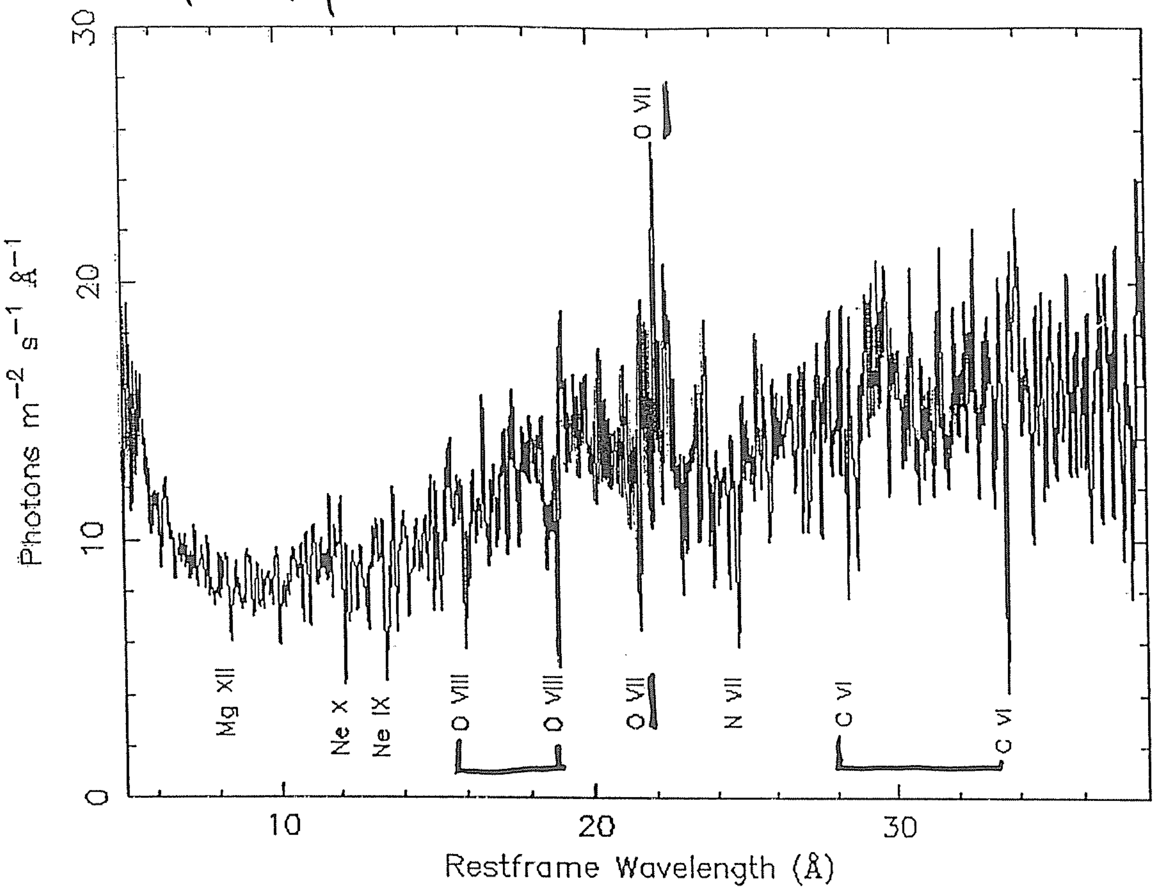
Ex: CCD spectrum of massive binary [BH/NS + WR star] Cyg X-3 (Kitamoto & al., 1994, PASJ, 46, L105):

Recombination radiation from X-ray photoionized wind of WR star

Same, Chandra HETGS (Paerels et al, 2000)



X-ray Absorption line Spectrum of Seyfert 1 Galaxy NGC 5548



Chandra LETGS, Kaastra & al., 2000:

1 deepest dips in noisy spectrum:
each coincides with strongest resonance transition n=1-2 in H, He-like
C, N, O, Ne, Mg

2 Absorption from every ion that should be there IS in fact detected

⇨ powerful principle:
SPECTROSCOPIC CONSISTENCY

Approximate Energies of Interest.

1. Nothing replaces the Bohr atom!

$$E_{nm} = Z^2 \cdot Ry \left(\frac{1}{n^2} - \frac{1}{m^2}\right) \quad ; Ry = 13.6\,eV$$

a) one-electron ions, resonance transitions (low densities → no population in excited states):

$$E_{1m} = Z^2 \cdot Ry \left(1 - \frac{1}{m^2}\right)$$

C VI Lyα	E = 367 eV	λ 33.8 Å
N	500	24.8
O	653	19.0
Ne	1020	12.16
Mg	1469	8.44
Si	2000	6.20
⋮		
Fe	6895	1.80

$$\left(E = hc/\lambda \rightarrow E = 12.3985/\lambda \, , \begin{array}{l} E : keV \\ \lambda : \text{Å} \end{array} \right)$$

⇨ abundant elements:

$\approx$ 350 → 2000 eV

Accurate transition Energies: Dirac Equation

(cf. Bethe & Salpeter: "QM of one and two electron atoms"; Sakurai: "Advanced QM")

Simple order of magnitude estimate: relativistic corrections to energies:

$$E^2 = E_0^2 + p^2c^2 \qquad (E_0 \equiv mc^2)$$

$$\Rightarrow \quad E \cong E_0\left(1 + \frac{p^2c^2}{2E_0^2} - \frac{1}{8}\left(\frac{p^2c^2}{E_0^2}\right)^2\right)$$

$\Rightarrow$ successive orders of approximation smaller by $\sim p^2c^2/E_0^2 = \frac{Z^2\alpha^2}{n^2}$

↑

(Bohr atom)

➡ $Z^2\alpha^2 = 1.9 \times 10^{-3}$ for C, already!

one-electron ions [cont'd]:

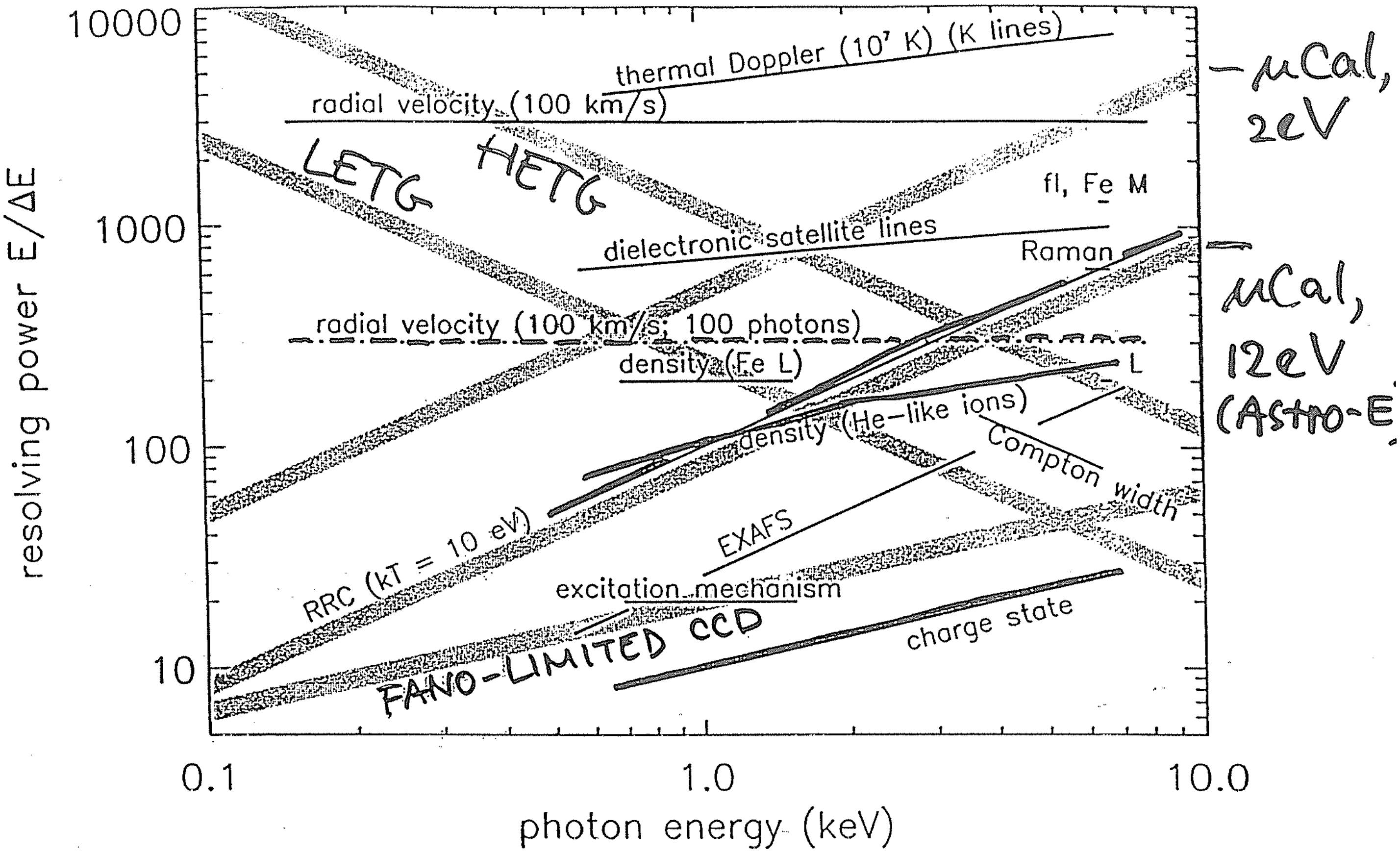
Also: l, s degeneracy lifted

→ see "Hβ" in Fe XXVI in Cyg X-3 !

Useful numbers for Ly-series:

- use solution to Dirac equation for H-like ions
- Tables compiled by Masao Sako
  (masao@astro.columbia.edu ;
  masao@astro.caltech.edu after Sep 1, 2001)

Different Types of Spectrometer
(a salespitch for gratings)



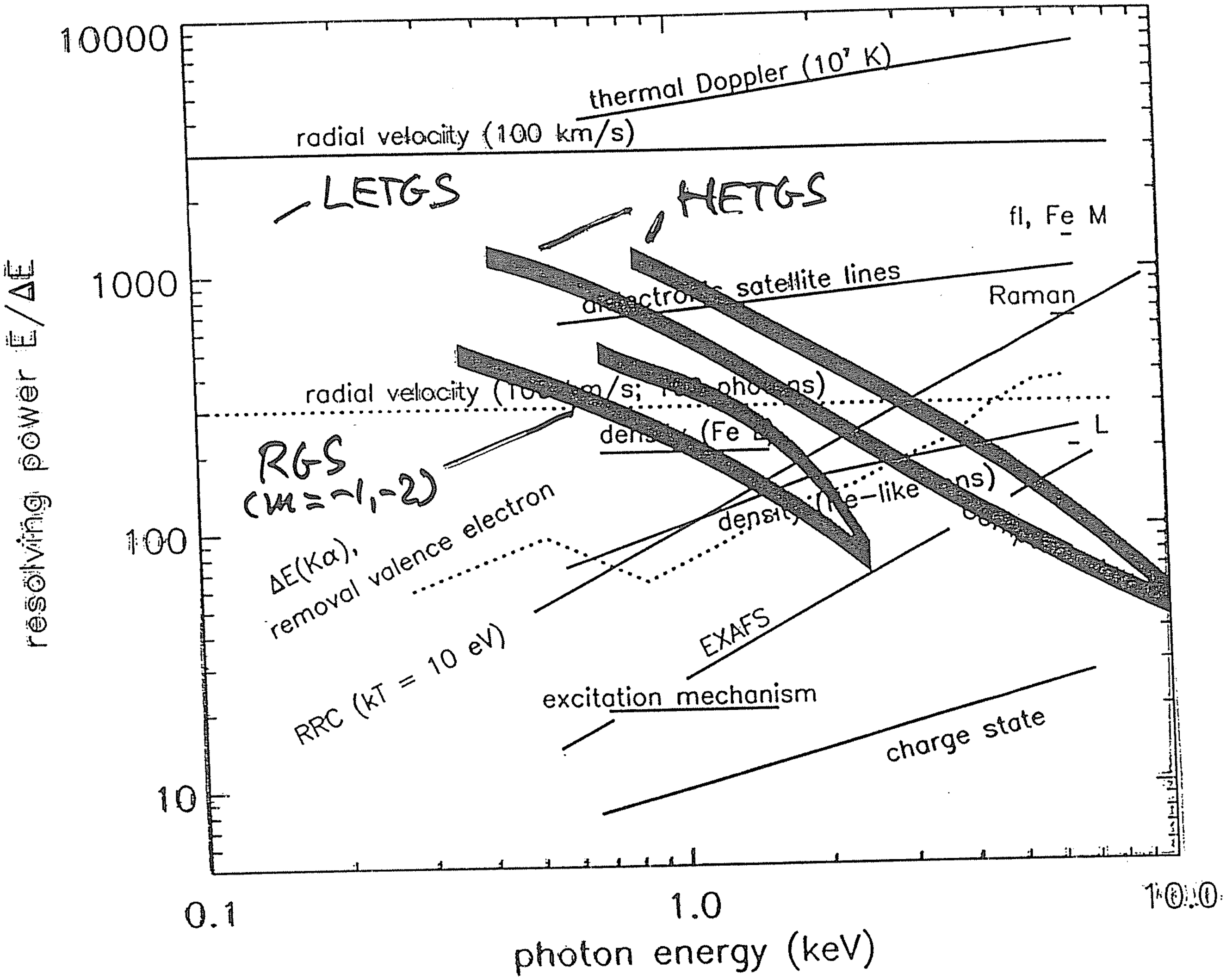
① Ionization detectors (prop counters, CCD's):
natural energy scale: ionization energy
⇒ $\Delta E \propto E^{1/2}$

② Microcalorimeters: ΔE = constant
(Quantum physics of lattice heat capacity)

③ Grating spectrometers: $\Delta\lambda \simeq$ constant
(<u>no</u> fundamental limit)

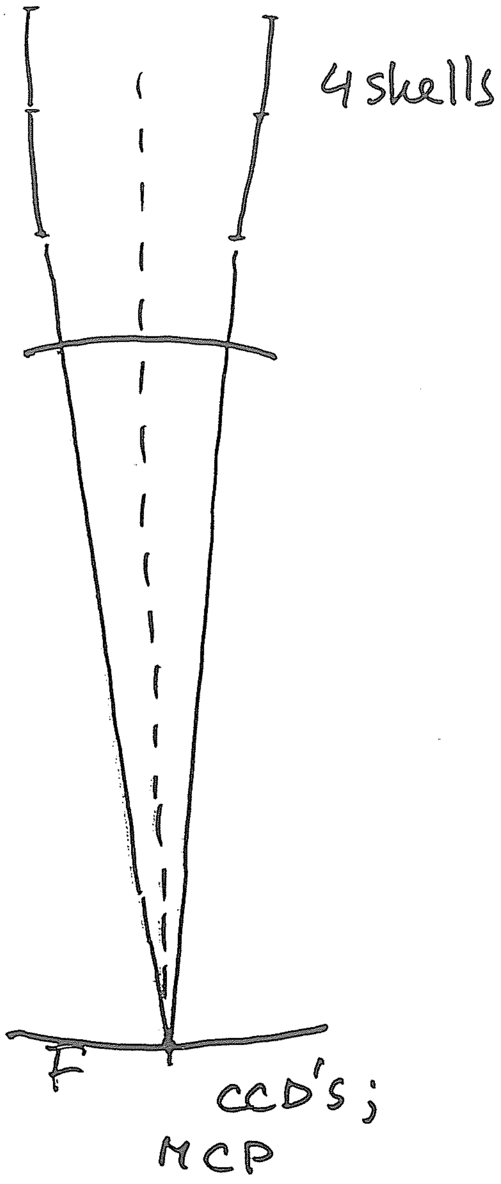
⇒ Gratings always beat CCD's, micro-calorimeters at low energies!

Real Resolving Powers : Diffraction Grating Spectrometers on Chandra, XMM-Newton

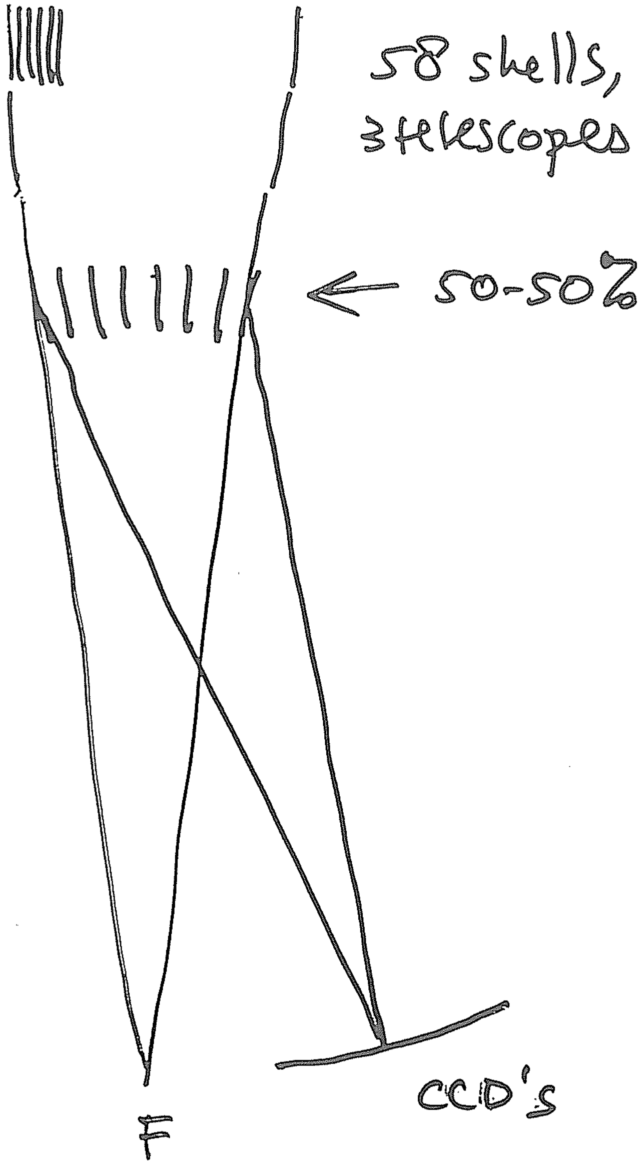


Chandra	XMM-Newton
Telescope $\Delta\theta \lesssim 1''$	$\Delta\theta \sim 8\text{-}10''$
transmission gratings: $R = \frac{\lambda}{\Delta\lambda} = \frac{\theta}{\Delta\theta}$ R large because $\Delta\theta$ small	Reflection Gratings: $\Delta\lambda = \frac{d}{m} \sin\alpha \cdot \Delta\theta$ grazing incidence $\Rightarrow \underline{\sin\alpha \sim 1/50}$ compensates for bigger $\Delta\theta$
$R \gtrsim 1000$	$R \gtrsim 500$ (300 at 15 Å)
A_{eff} ($E \lesssim 2$ keV) < 100 cm^2 ($\to 10$ cm^2)	A_{eff} ($E \lesssim 2$ keV) ~ 100 cm^2
Superior performance at $E > 2$ keV	band limited to 0.3 – 2.5 keV ($E > 2$ keV: CCD's)
resolution degrades $\Delta\varphi \gtrsim 1$ arcsec	resolution degrades $\Delta\varphi \gtrsim 30''$: moderately extended sources.
either imaging OR grating spectroscopy	RGS always in (but the light is

Chandra



XMM-Newton



Both "slitless" spectrometers:
spectral/spatial coupling along dispersion direction

Discrete Transitions : quick recapitulation

- Atomic structure multi-electron systems:

$$H = H_{\text{central field}} + \text{electrostatic e-e} + \\ + \text{spin-orbit} + \dots$$

$$\equiv H_0 + H_{\text{pert}}$$

Electrostatic interactions:

$$\left.\begin{array}{l} \sum \vec{l}_i \equiv \vec{L} \\ \sum \vec{s}_i \equiv \vec{S} \end{array}\right\} \text{conserved}$$

$\Rightarrow$ L, S good quantum numbers

(non-relativistic, electrostatic interactions only!)

Labeling:

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

$L = 0, 1, 2, \dots$: "S, P, D, F, ...

e.g. (simplest example):

H in $n=2$, $l=1$: ^2P

Radiative Transitions:

Semiclassical (EM field classical);

First-order perturbation theory:

transition probability $i \to f$:

$$\propto |\langle f| H_{fi} |i\rangle|^2$$

H_{fi}: induces the transition (interaction energy):

$$H_i = \frac{1}{2m}(\vec{P}_i - \frac{e}{c}\vec{A}) + e\varphi =$$

$$= \frac{P_i^2}{2m} + e\varphi - \underset{\underset{\text{one photon}}{\uparrow}}{\frac{e}{mc}\vec{A}\cdot\vec{P}_i} + \underset{\underset{\text{two photon}}{\nwarrow}}{\frac{e^2A^2}{2mc^2}}$$

Set $\vec{A}(\vec{r},t) = \vec{A}(t)\, e^{i\vec{k}\cdot\vec{r}}$ (plane wave)

$$\Rightarrow H_{fi} = \bar{A}(\omega_{fi}) \frac{ie\hbar}{mc} \langle f| e^{i\vec{k}\cdot\vec{r}} \underset{\underset{\text{electron momenta}}{\uparrow}}{\sum_i \nabla_i} |i\rangle$$

- Dipole Approximation:

$$e^{i\vec{k}\cdot\vec{r}} = \underset{\substack{\uparrow \\ \text{dipole approximation}}}{1} + i\vec{k}\cdot\vec{r} + \frac{1}{2}(i\vec{k}\cdot\vec{r})^2 + \dots$$

because $|H_{fi}|^2 \propto |d_{fi}|^2$

Higher order terms smaller by

$$\vec{k}\cdot\vec{r} \sim k a_0$$

$$\sim \frac{\text{size atom}}{\text{radiation wavelength}}$$

$$\sim Z\alpha$$

$$\sim v/c \qquad \ll 1 \text{ in dipole approximation}$$

(and probability $\propto |\vec{k}\cdot\vec{r}|^2$)

Nomenclature:

Electric Dipole, E1, "dipole allowed"

$\left\{ \begin{array}{l} \text{Electric Quadrupole (E2),} \\ \text{Magnetic Dipole (M1),} \end{array} \right.$

Electric Octupole ....

Spontaneous Transition Rate A_{ji}

(from induced rate & relation A, B) :

$$A_{ji} = 6.7 \times 10^{15} \frac{w_i}{w_j} f_{ij} \lambda_{\text{Å}}^{-2}$$

$f_{ij} \sim 1$, constant

$$\Rightarrow \underline{A_{ij} \propto Z^4}$$

- symmetry properties of $\langle f | e^{i\vec{k}\cdot\vec{r}} \nabla_i | i \rangle$ give rise to selection rules.

  E1 transitions :

  $\Delta L = 0, \pm 1$

  $\Delta S = 0$

  $\Delta J = 0, \pm 1$; $\cancel{J = 0 \to J = 0}$

  $\cancel{M_J = 0 \to M_J = 0}$

- Other Processes (e.g. collisions with charged particles) : same idea.

Example : "spin-flip" transitions

"proton spin-flip" in superstrong $\vec{B}$-field

- $B \sim 10^{15}$ G (so-called "magnetar", strongly magnetized young NS)

- circular orbits charged particles in $\vec{B}$-field quantized ("Landau levels"):

$$E_n = (n + \tfrac{1}{2})\hbar\omega_B =$$

$$= (n+\tfrac{1}{2})\hbar \frac{qB}{m_p c} \Rightarrow$$

$$\Delta E = 6.3 \left(B/10^{15} G \right) \text{keV}$$

- $$\frac{\text{probability spin flip}}{\text{probability } \Delta n = 1} \sim \left(\frac{v}{c}\right)^2$$

$$\sim \frac{\Delta E}{m_p c^2} = \frac{6.3 \, B_{15}}{511 \times 1836} \ll 1$$

→ very weak transition

Example: He-like ions $n = 1-2$

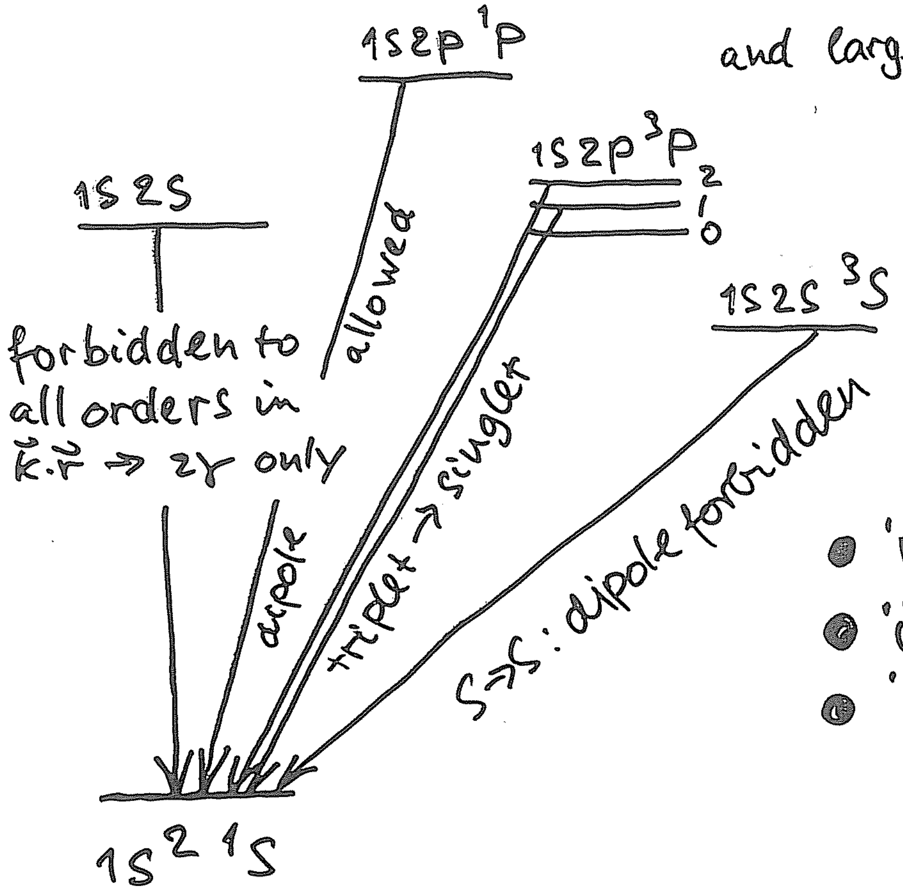
two electrons : eigenfunctions of $|\vec{S}_{total}|^2$:

$\uparrow\uparrow, \downarrow\downarrow, \uparrow\downarrow + \downarrow\uparrow$: triplet

$\uparrow\downarrow - \downarrow\uparrow$: singlet

total wavefunction must be antisymmetric

spin anti → space symmetric
← Pauli : e's close, $\Delta E_{electrostatic} > 0$
and larger than triplet states



- 'resonance' w
- 'intercombination' x, y
- 'forbidden' z

He-like ions are IMPORTANT in X-ray astronomy!

Astrophysical Plasmas

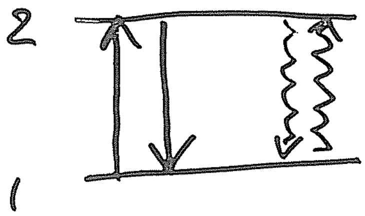
- low density ; high ionization
- optically thin (ignore radiative transfer)
- (● f(v) Maxwellian)

⇒ radiation excited in source escapes freely ;
spectrum directly reflects physical conditions at the source

(velocities, density, temperature, ionization balance, degree of equilibration, ...)

- examples : hot gas stellar coronae, SNR, ISM, clusters, IGM ; highly ionized gas in accretion flows, GRB Afterglows (?), ...

- what is 'low' density ?



collisional ↓ rate >> spontaneous decay rate :

⇒ MEDIUM in LTE : thermal energy / radiation field very

(i.e. continuous conversion
thermal energy gas $\leftrightarrows$ radiation)

[NB: if radiative transitions dominate,
$\Rightarrow$ TE if $I_{12} \rightarrow B_{12}(T)$, i.e. if $\tau_{12} \ggg 1$]

n "low" if

$$\boxed{A_{21} \gg n_e C_{21}(T_e)}$$

$$\Rightarrow \quad n_e \gtrsim 1.4\times10^{15}(Z+1)^6 T^{1/2} \text{ cm}^{-3}$$

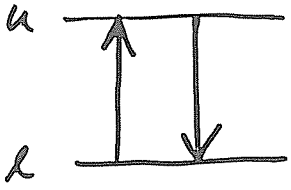
- If n_e "low":
  - most ions in $n=1$
  - excitations followed by production of photon
  - ionization balance $\neq$ Saha, but found from rate equations

(sometimes referred to as "coronal approx.", but also applies to low density radiation dominated plasma's)

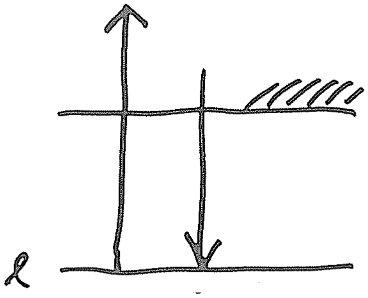
Most Common Interactions between electrons, ions, and photons:

1. Compton scattering on free or bound e^-'s

2.

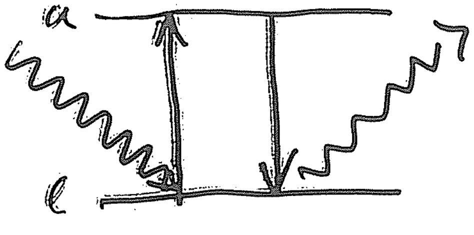


collisional excitation/
deexcitation

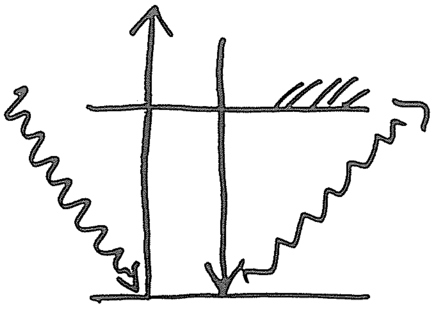


collisional ionization/
3-body recombination
($1e^-: f \to f$, $1e^-: f \to b$;
plus ion)
3BR only at high densities!

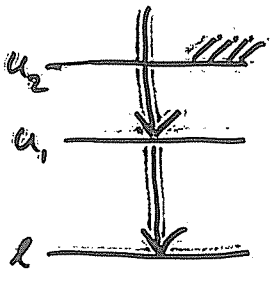
3.



photoexcitation;
(photon can be line or <u>continuum</u>); radiative decay.



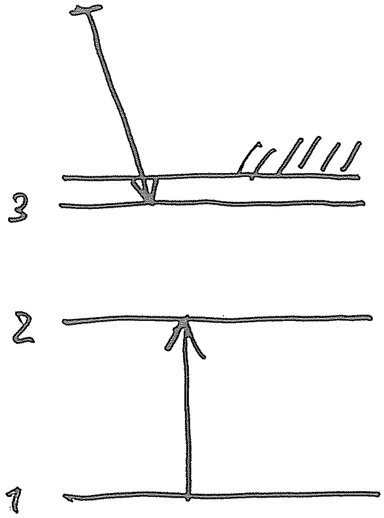
photoionization;
radiative recombination



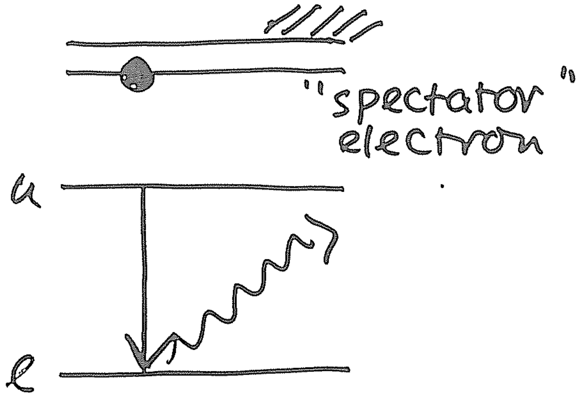
"cascade"

If $l = 1, u = 2$: "resonance line" $n = 1$-2;
photon can not be destroyed & scatters

4.



⇒

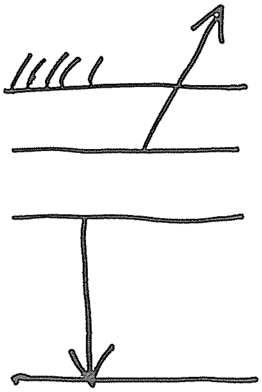


dielectronic recombination

(if "3" in continuum:
"resonant excitation")

"satellite line"
(close to $u \to l$
in ion $Z+1$)

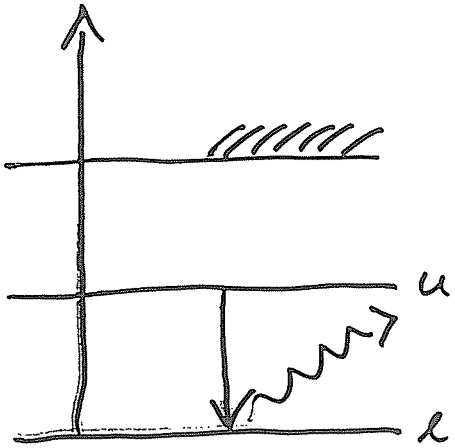
OR



Auger ionization

(either CI or PI)

5.



or Auger; no
photons, only
electrons

fluorescence
$y \cong (Z/26)^4 \times 0.3$

cross-sections:
cf. compilation in
Mewe (1998)

4. IONIZATION BALANCE.

Roughly speaking, two types of high ionization plasma:

$$\begin{cases} \text{collisionally ionized} & : kT_e \sim \chi \\ \text{photoionized} & : kT_e \ll \chi \end{cases}$$

(Mixed type, if radiation energy density high, and also $kT_e \sim \chi$).

4.1 collisionally ionized gas (a.k.a. "coronal plasma", or just: "hot gas")

- thermal balance:
  heat in = radiation out
- ionization balance:

$$\frac{dn_i}{dt} = +n_e n_{i-1} C_{i-1,i} + \\ + n_e n_{i+1} \alpha_{i+1,i} - \\ - n_e n_i (C_{i,i+1} + \alpha_{i,i-1})$$

Calculations:

- approximate expressions in Mewe ('98)
- calculations: Arnaud & Rothenflug, 1985, A&A Suppl., 60, 425
- Fe L: Arnaud & Raymond, 1992,

NB Auger ionization couples ions several stages apart! (not shown in dn_i/dt)

Balance is between direct collisional ionization, and RR + DR

$\uparrow$ important at low T due to resonant character of process

➡ non-equilibrium ionization:

$$\frac{dn_i}{dt} \neq 0 \quad ;$$

characteristic timescale : $\frac{1}{n_e \alpha}$, $\frac{1}{n_e C}$

Approximate expressions:

$$n_e t_{ion.} \approx 10^{10} (Z+1)^4 n_Z^{-4} \xi_Z^{-1} T^{-1/2} e^{Y} \quad [\mathrm{cm}^{-3}\,\mathrm{s}]$$

$\uparrow$ charge

$\uparrow$ principal quantum # valence shell

$\uparrow$ nr. valence electrons

$$y \equiv 1.6 \times 10^5 (Z+1)^2 n_Z^{-2} T^{-1}$$

$$n_e t_{rec.} \approx 10^{11} (Z+1)^{-2} n_Z^{5/2} \xi_Z^{-1} T^{1/2} \quad [\mathrm{cm}^{-3}\,\mathrm{s}]$$

$\uparrow$ nr. holes in valence shell

(Mewe ['98])

Examples:

- He-like → H-like O at $T = 5.10^6$ K :

  $(n_z = 1, z = 6, \xi_z = 2, y = 1.6)$

  $\rightarrow n_e t_{ion} \cong 2.6 \times 10^{10}$ cm^{-3} s

  ISM, $n_e \sim 1$: $t_{ion} \sim 800$ yrs!

  so SNR, $t < t_{ion}$: under ionized

- stripped → H-like O at $T = 10^8$ K :

  $(\xi_z = 2, n_z = 1, z = 8)$

  $\rightarrow n_e t_{rec} \simeq 6.10^{12}$ cm^{-3} s

  GRB: afterglow-illuminated ejecta:
  If you detect bound O 1 day after the burst : $t_{rec} \lesssim 10^5$ sec

  $\Rightarrow n_e \gtrsim 6.10^7$ cm^{-3}

4.2 X-ray Photoionized Gas

- energy balance :

  photoelectric, Compton heating +
  whatever else =
  = radiative cooling

- ionization balance :

$$\frac{dn_i}{dt} = -n_i \int_{\chi}^{\infty} dE\, \sigma(E)\, \frac{F(E)}{E} + n_{i+1} n_e \alpha(T)$$

(only 2 stages shown)

1: thermal balance & ionization balance COUPLED (through $\alpha(T_e)$) [UNLIKE collisional plasma's]
explicit solutions: $\boxed{kT_e \ll \chi}$ $\underline{\underline{\text{COOL}}}$

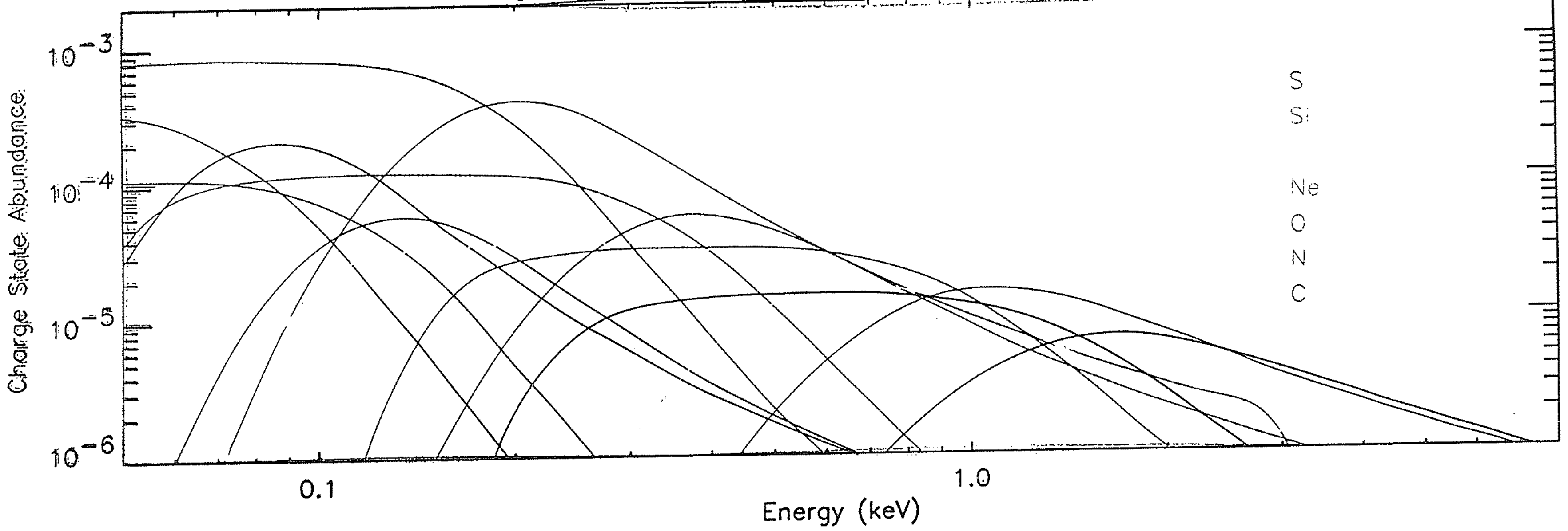
(Kallman & McCray, 1982, ApJ Suppl. <u>50</u>, 263)
⇒ XSTAR code
Gary Ferland ⇒ CLOUDY
Hagai Netzer ⇒ ION ; & others)

2: degree of ionization scales with $\underline{\xi}$:
in equilibrium:

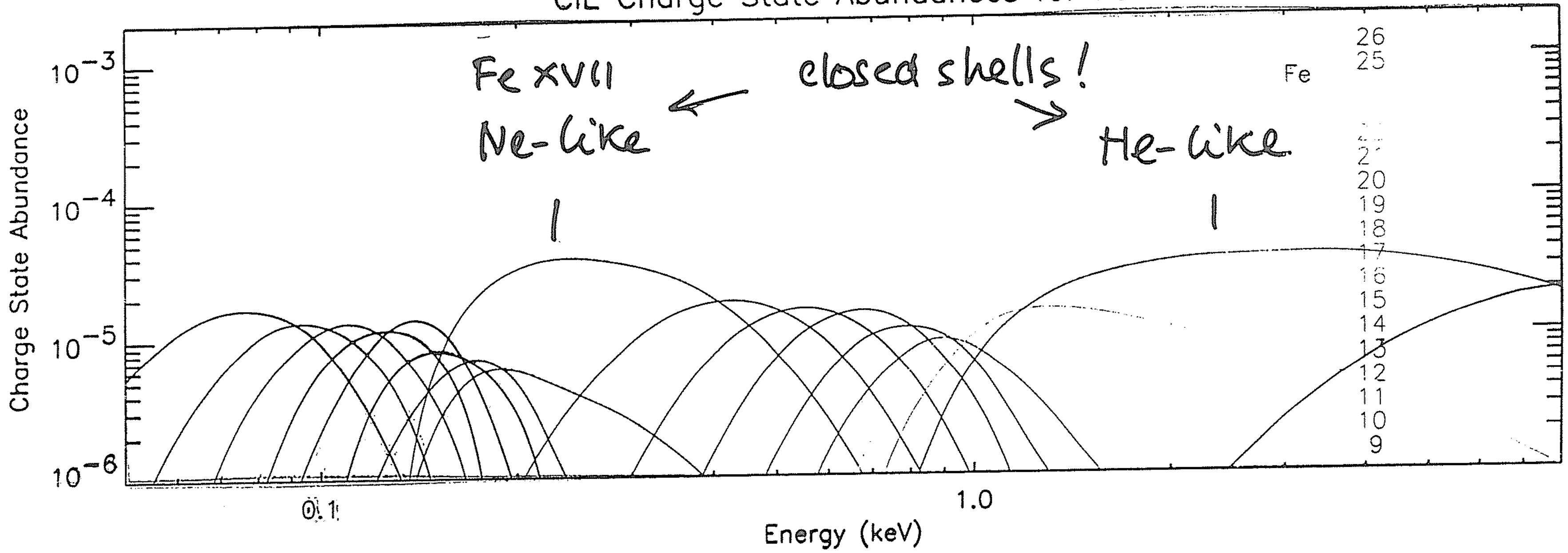
$$\frac{n_{i+1}}{n_i} = \underbrace{\boxed{\frac{L}{n_e r^2}}}_{=\,\xi} \times \frac{1}{4\pi}\, \frac{\int_{\chi}^{\infty} dE\, \sigma(E)\, f(E)\cdot E^{-1}}{\alpha(T_e)}$$

COLLISIONAL IONIZATION EQUILIBRIUM

CIE Charge State Abundances for H- and He-like Species



CIE Charge State Abundances for Fe



Fe XVII

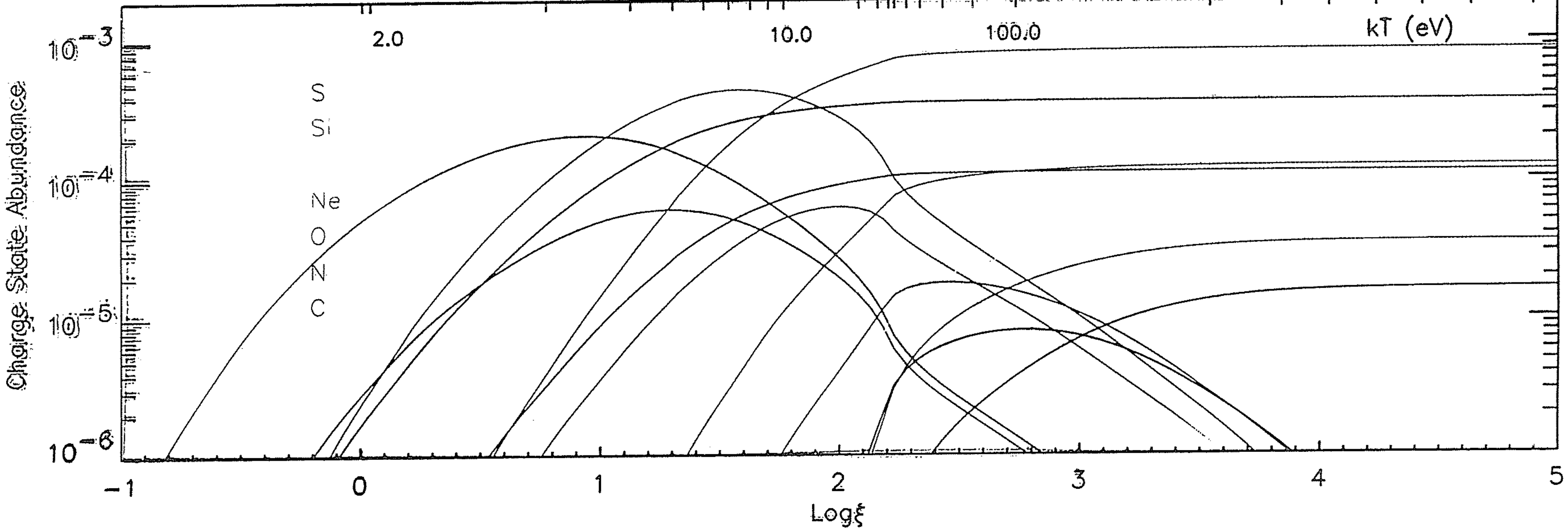
Ne-like ← closed shells! → He-like

(i.e. electron temperature)

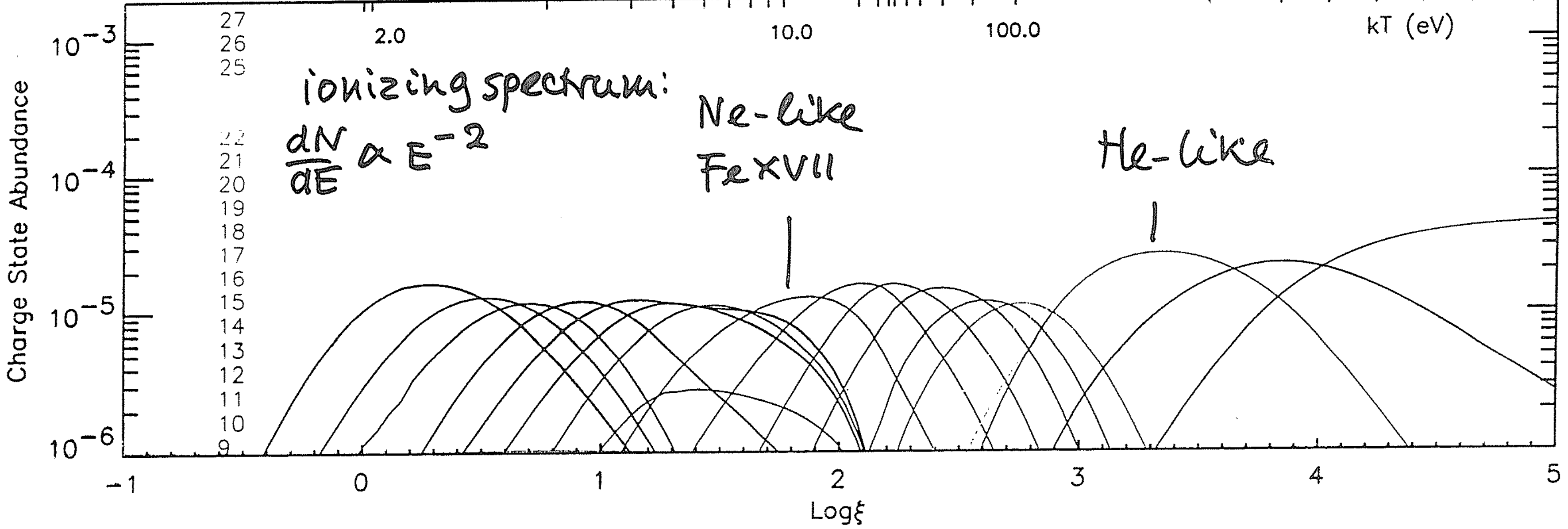
Ref: Arnaud, M. and Rothenflug, R. 1985, A&AS, 60, 425

PHOTOIONIZATION EQUILIBRIUM

PIE Charge State Abundances for bare and H−like Species (Γ=2.0)



PIE Charge State Abundances for Fe (Γ=2.0)



ionizing spectrum:
$\frac{dN}{dE} \propto E^{-2}$

Ne-like
Fe XVII

He-like

<u>NB</u>: ● collisional balance neatly sequential $n_i \to n_{i+1} \to n_{i+2}$

$$\xrightarrow[kT_e]{\qquad\qquad}$$

● photoionization balance more messy: multiple species simultaneously present (consequence of "flat" ionizing spectrum E^{-2}, as opposed to $f(v)$ [Maxwell])

➡ Fe L ions cover wide range in either kT_e, ξ : excellent diagnostics over wide range in conditions

Fun calculation: fluorescence line fluxes for different elements:

$$\text{fluorescence rate} = n \cdot y \cdot \int_{\chi}^{\infty} dE \cdot F_0 E^{-\Gamma} \sigma(E)$$

$$\sigma(E) \cong 6 \cdot 10^{-18} Z^{-2} (\chi/E)^3 \ \text{cm}^2 \ ;$$

set $\Gamma = 2$ (AGN, GRB afterglow)

$$\Rightarrow \ \text{rate} = n \cdot y \cdot F_0 \sigma_0 \cdot \frac{1}{4 Z^2 \chi}$$

Now, $\chi \propto Z^2$, so rate $\propto \frac{y}{Z^4}$; and since $y \propto Z^4 \Rightarrow$ rate = independent of Z!

5. Collisional Plasma's: Spectroscopy

1. Collisional excitation rate = photon emission rate (in our case)

   $\propto$ ion abundance × excitation rate [Mewe ['98])

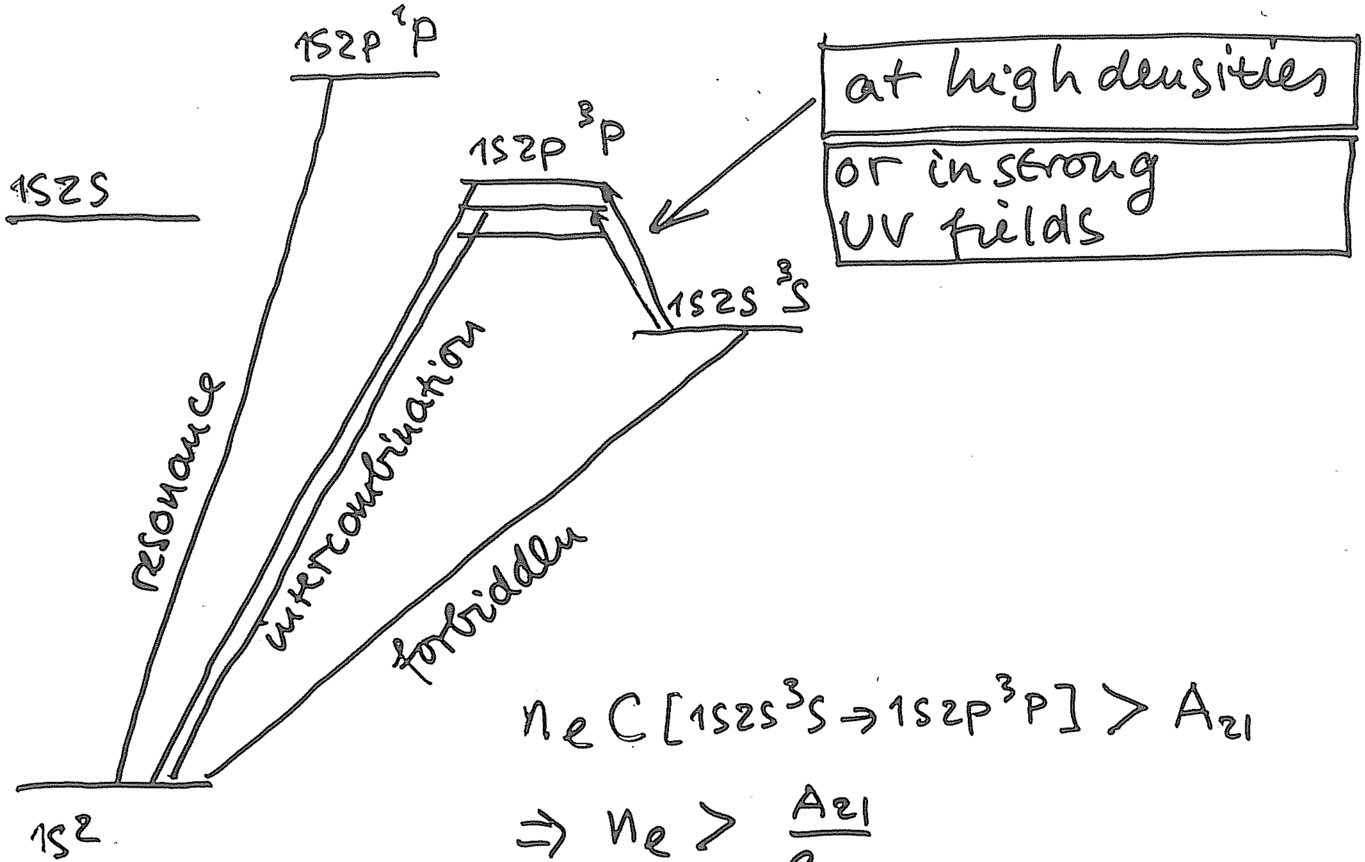
   ⇨ strongest dependence is in ionization balance

   ⇨ strongest T-diagnostic from ionization balance (unfortunately — involves a lot of explicit rate coefficients)

   ⇨ emission spectra individual ions NOT very sensitive to T_e, in T_e-range where ion observable [ionization balance!], except in unusual circumstances

   ex: He-like ions placed in very high T_e (compared to equilibrium ionization balance):
   emission line ratio's sensitive at high T_e - cf. Andy Rasmussen et al., 2001, A&A, 365)

2. Density sensitivity He-like n=1-2 emission spectrum



$n_e C[1s2s\,^3S \rightarrow 1s2p\,^3P] > A_{21}$

$\Rightarrow n_e > \frac{A_{21}}{C_{22}}$

collisional transfer faster than spontaneous decay (easy, because A_{21} forbidden)

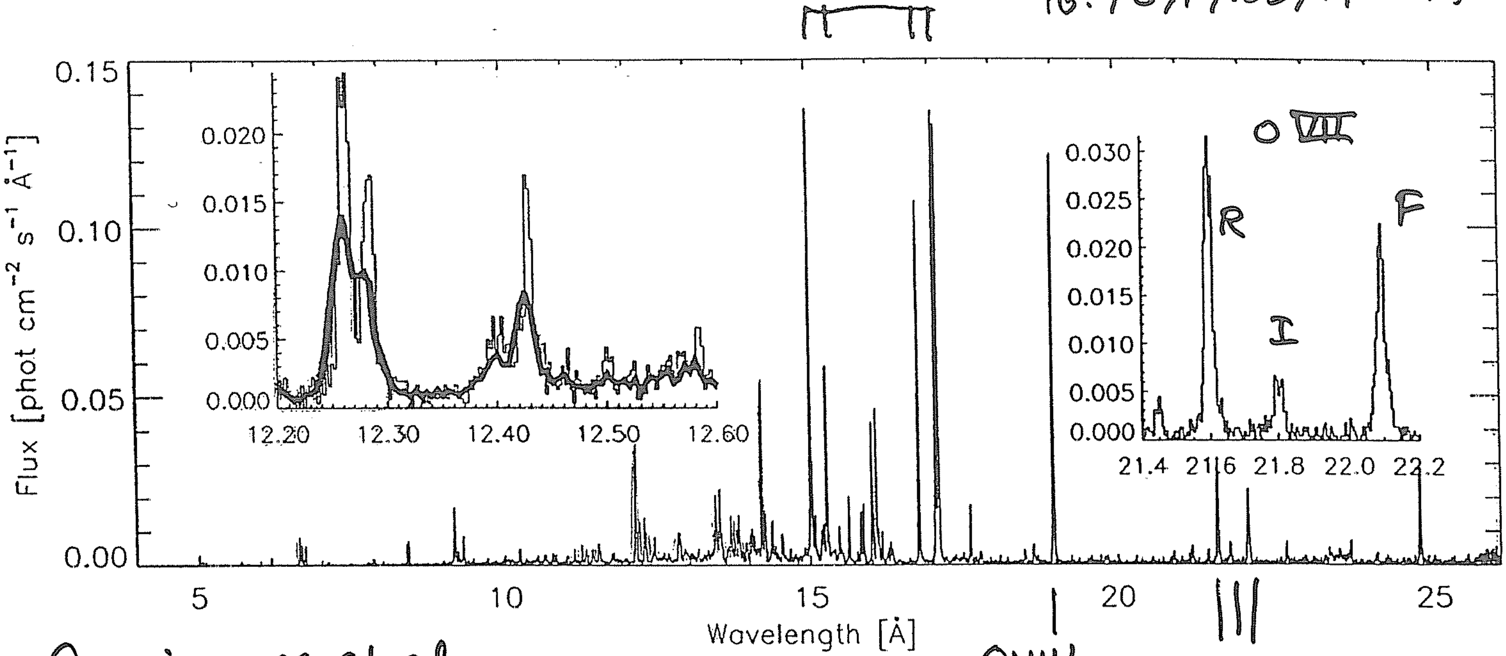
- $n_{e,crit}$ depends on Z; ranges ~$10^8 - 10^{12}$ cm^{-3}
  C – Si

- get upper limit if F strong; real measurement if $n_e \gtrsim n_{e,crit}$

- radiative transfer: O stars, accretion disks

Example: HETGS spectroscopy of coronae in Capella

Fe XVII 15.014, 15.26, 16.78, 17.05, 17.10 Å



O VIII Lyα

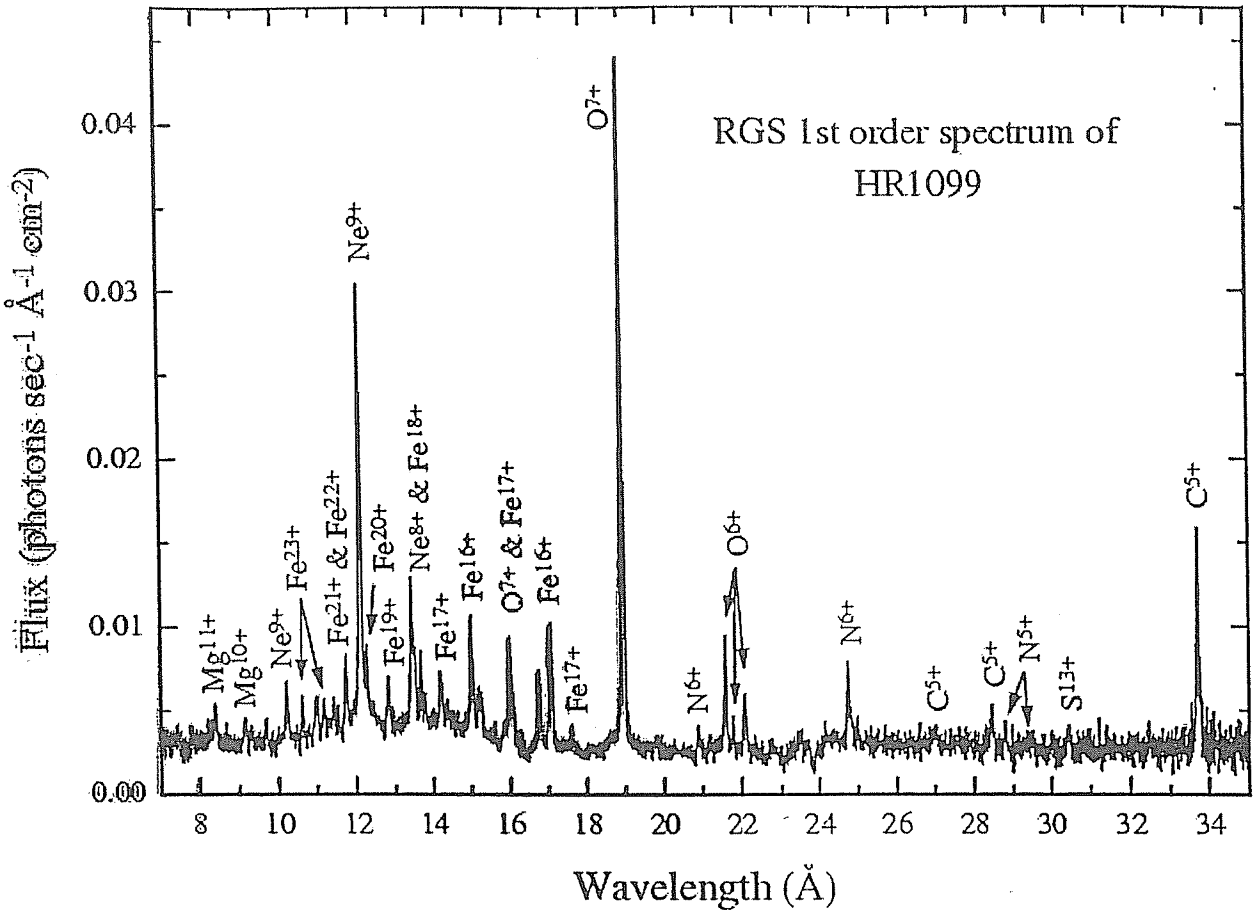
O VII

Canizares et al., 2000, ApJ, 539, L41.

↑ dominated by Fe L

- He-like O: $n \sim n_{crit}$!
- T-distribution from ionization balance.

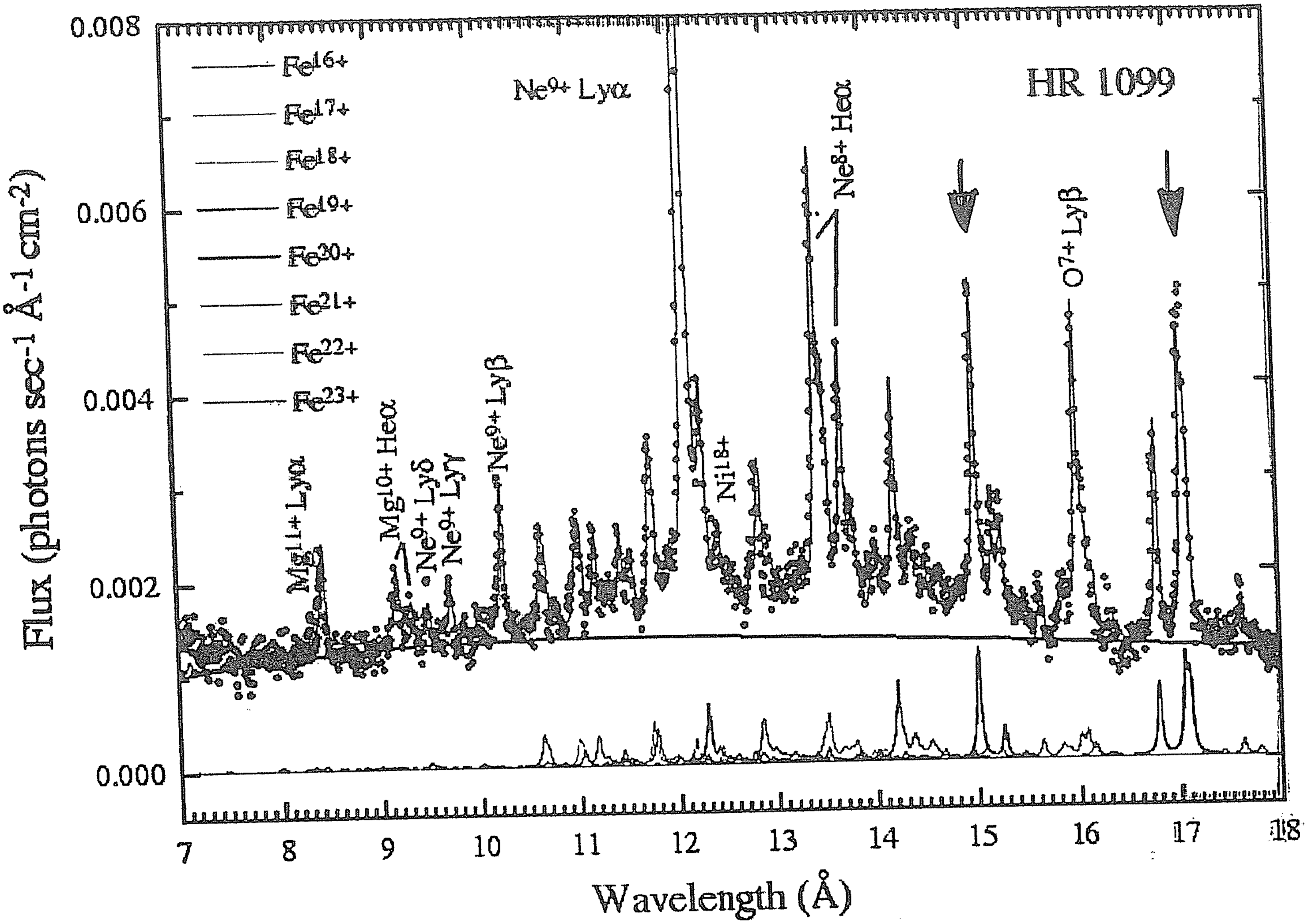
Similarly: HR1099 with XMM-Newton RGS



Brinkman & al., 2001, A&A, 365.

- → most FeL lines are $n = 2-3$ (2p-3d)
- → line strengths: direct excitation; tiny bit recombination into upper level; excitation to higher levels + cascading

How well can we quantitatively calculate emission from a collisional plasma?



(Brinkman & al, 2001; courtesy Ehud Behar)

- pretty close fit! some questions remain regarding emission line ratio's in Fe $\overline{\underline{XVII}}$
- various calculations/compilations:

"Raymond-Smith" → APEC
"MeKaL" = Mewe / Kaastra / Liedahl
(NB public version not fully up to date)
Ehud Behar @ Columbia

ALL: IONIZATION BALANCE ⊗ COLLISIONAL RATES

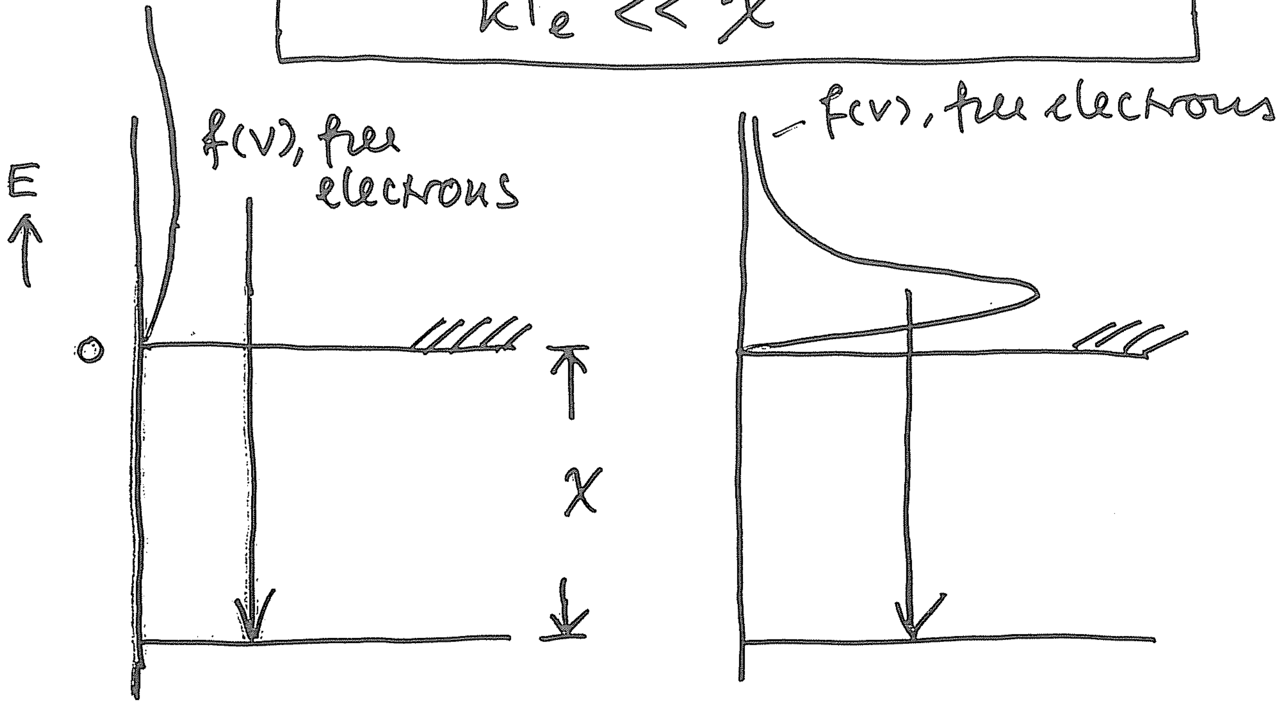
6. PHOTOIONIZED PLASMA'S: DIAGNOSTICS.

- inherently more complicated than collision-dominated case:
  - ① thermal + ionization balance coupled
  - ② ionization balance needs large amount of DR rate data (NB: plasma cool: DR very important)
  - ③ emission line power: have to solve rate equations for all cascades following recombination into excited states.
  - ④ by its very nature: radiative transfer much more likely to be important!
- Unusual individual diagnostics (no terrestrial experiments! cf. Tokamaks, Atomic bombs)

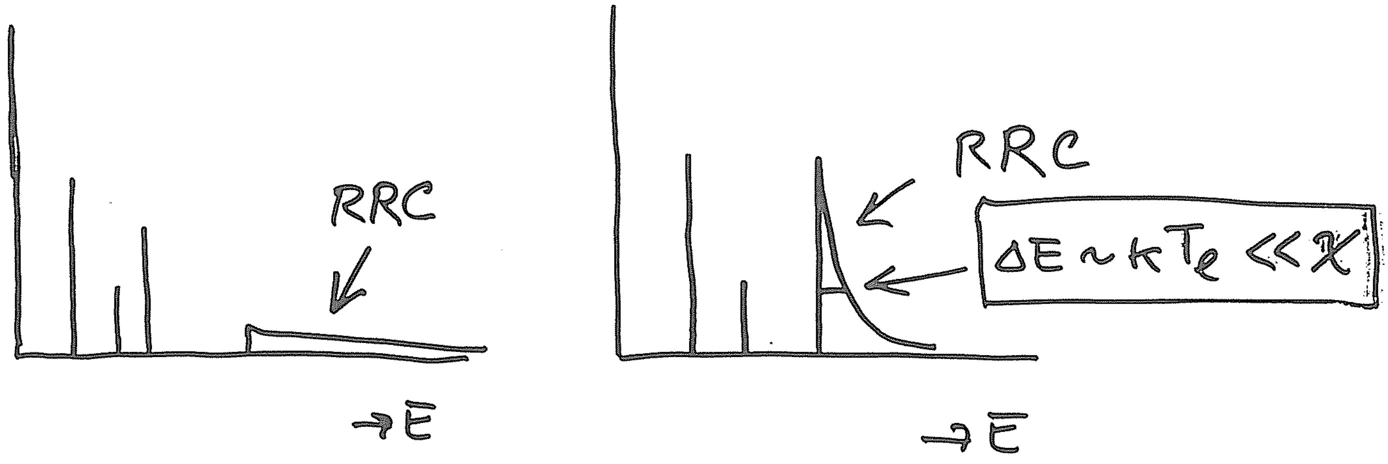
⇨ but collisional & recombination spectra easy to distinguish!

diagnostic 1: kT_e directly

photoionized gas is COOL:
$kT_e \ll \chi$



COLLISIONAL PHOTOIONIZED

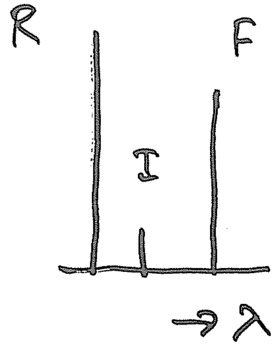


- seen in SN1987A (Balmer jump; gas has cooled substantially)
- reinvented by Duane Liedahl (priority goes to Dick McCray)
- and subsequently seen in X-rays in Cyg X-3

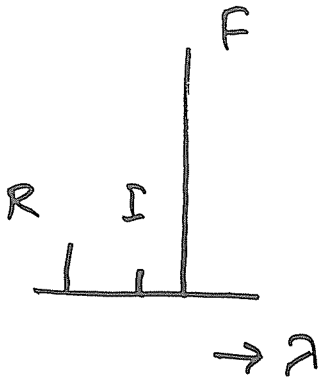
diagnostic 2:

- He-like ions: <u>recombination: F >> I, R</u>

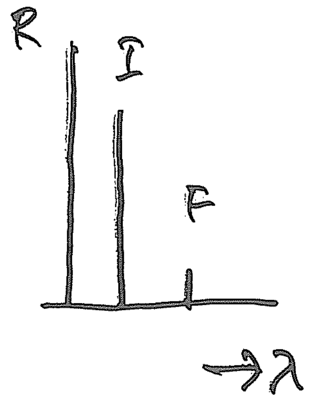
collisional



recombination

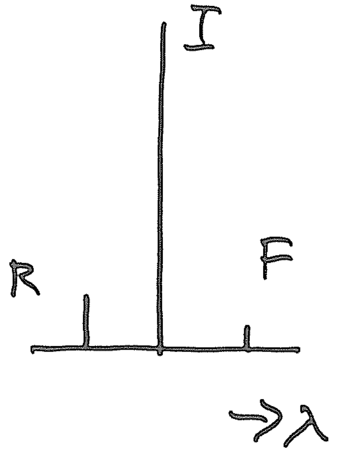


- density diagnostic still operates!



$n_e >> n_{crit}$:

F → I



⇑

seen in LMXB spectra:
Jean Cottam et al., 2001,
A&A, 365
(EXO 0748, 4U1822)

diagnostic 3:

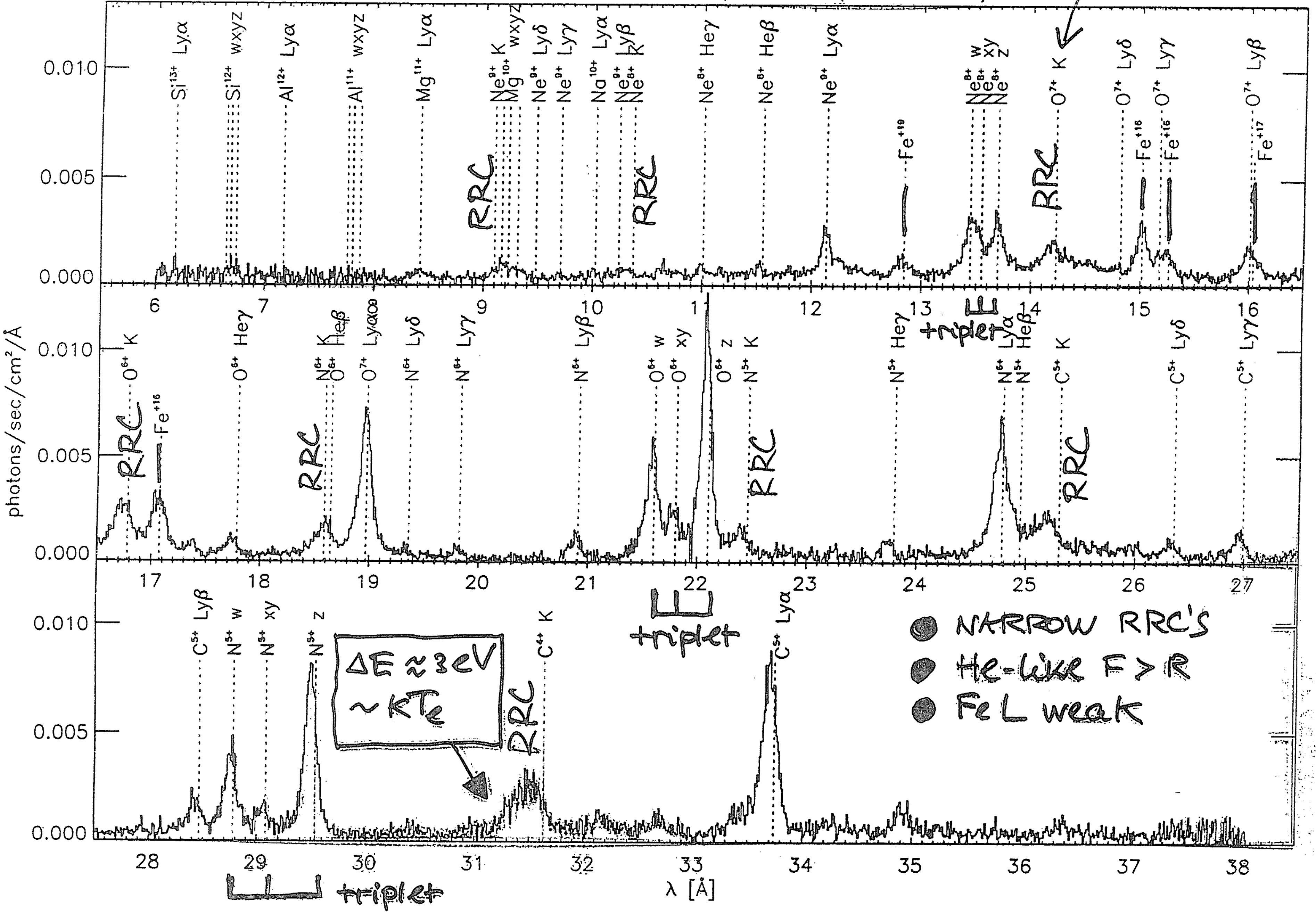
- Fe L recombination power << collisional power
  ⇒ low Z K shells BRIGHTER than Fe L

XMM/RGS 1
FIRST ORDER

DOMINATED BY PHOTOIONIZATION

$kT_e \approx 3eV$

NGC1068 Rest-Frame Spectrum (z=0.00379)



$\Delta E \approx 3eV$
$\sim kT_e$

- NARROW RRC'S
- He-like F > R
- Fe L weak

+ RGS 2! (lack of space)

7. OTHER DIAGNOSTICS & FUN STUFF

- collisional gas : coronae, SNR, ISM,
  clusters, IGM (?)
- recombination dominated spectra:
  → accretion dominated sources
  (XRB, AGN)

? Radiative transfer effect (resonance scattering) in strong emission lines from hot gas in clusters
$\Rightarrow H_0, D_A$ without SZ!

? GRB afterglow spectroscopy : weak evidence for Fe K; excitation mech. unknown ⇒ X-ray redshifts; chemical composition → ~~progenitor~~?

? Dense plasmas : neutron star atmospheres, M-R relation

? Absorption spectroscopy IGM ?

? Find the warm IGM in emission w/ narrow-band imaging?

⋮