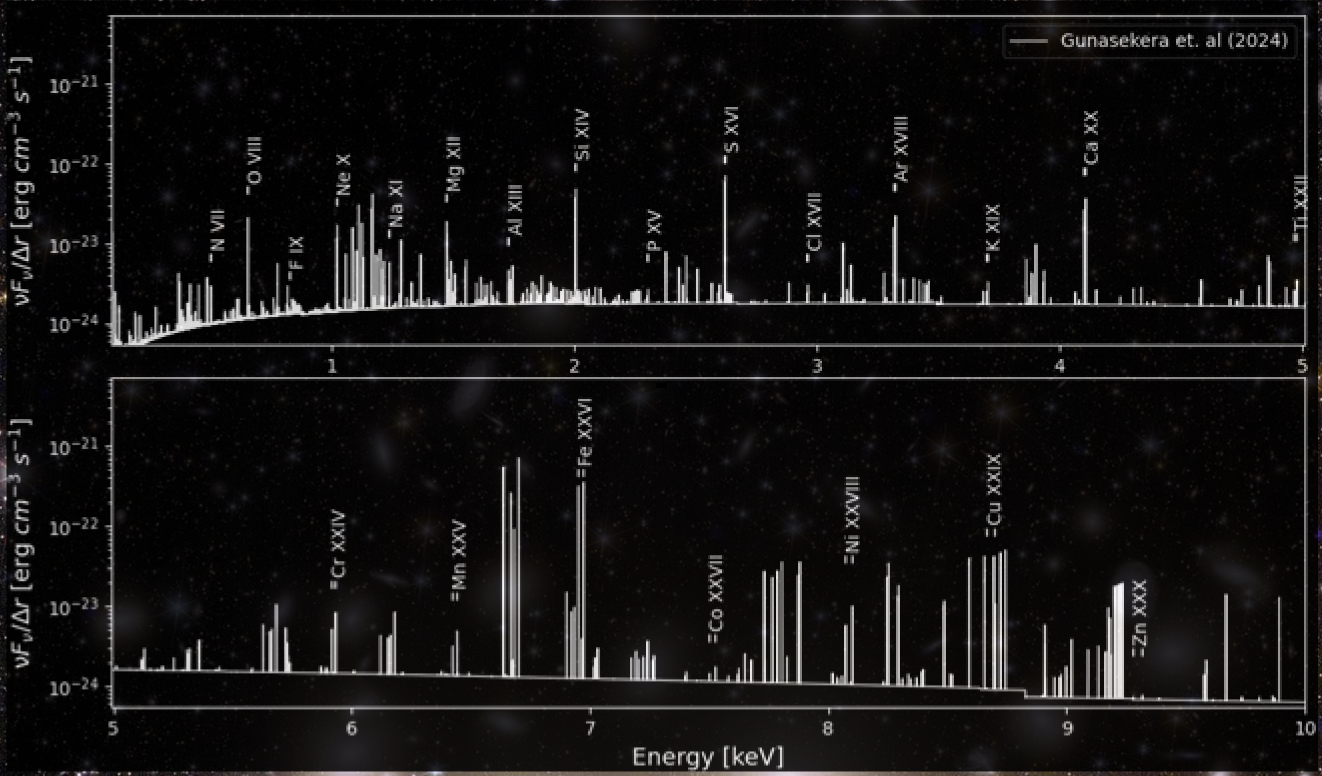
Preparing for High-Resolution X-rays in the Microcalorimeter Era



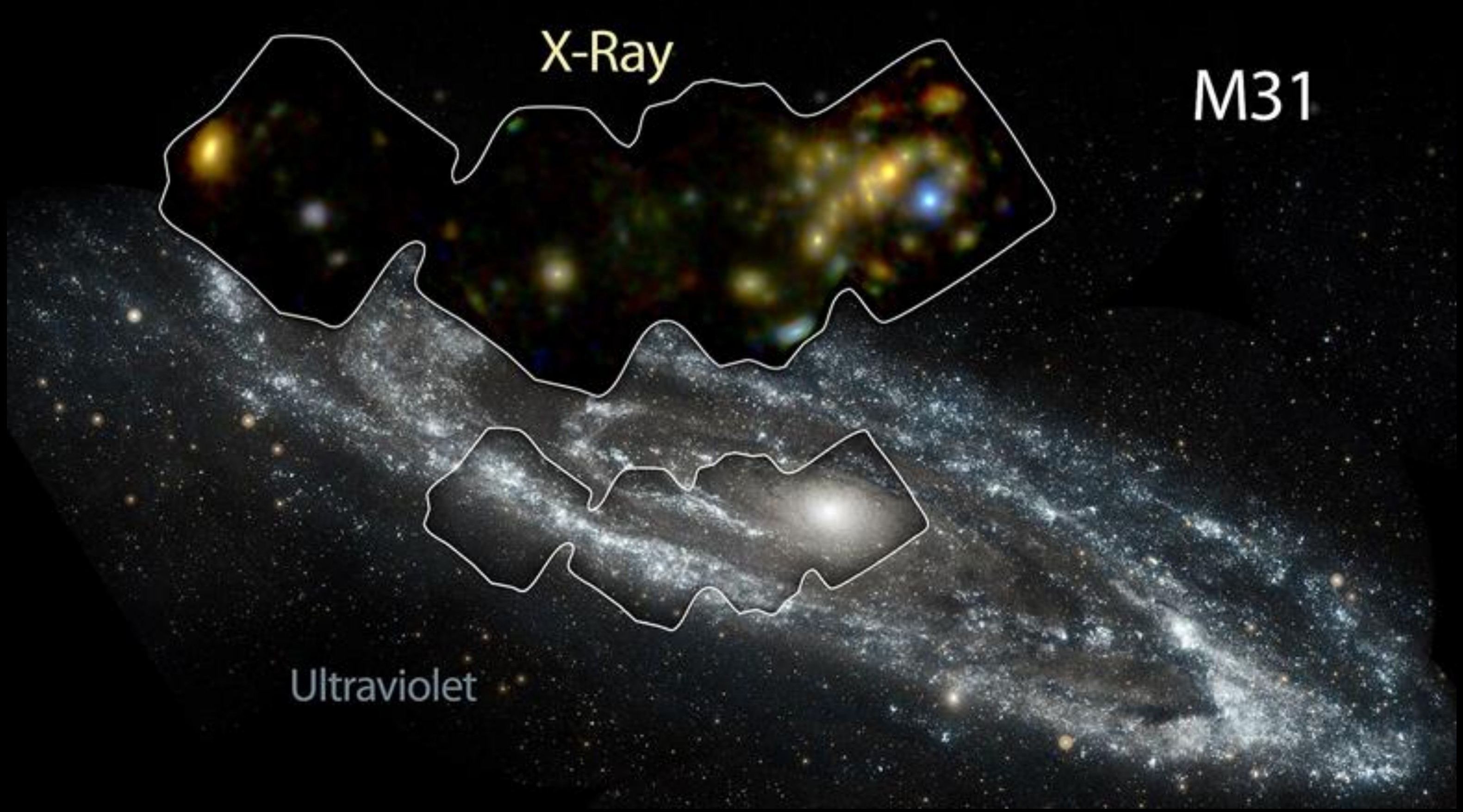
Chamani Gunasekera

Collaborators:

Peter van Hoof, Masahiro Tsujimoto, Stefano Bianchi, Marios Chatzikos, Gary J. Ferland

STScI | SPACE TELESCOPE SCIENCE INSTITUTE

Our Universe in X-ray



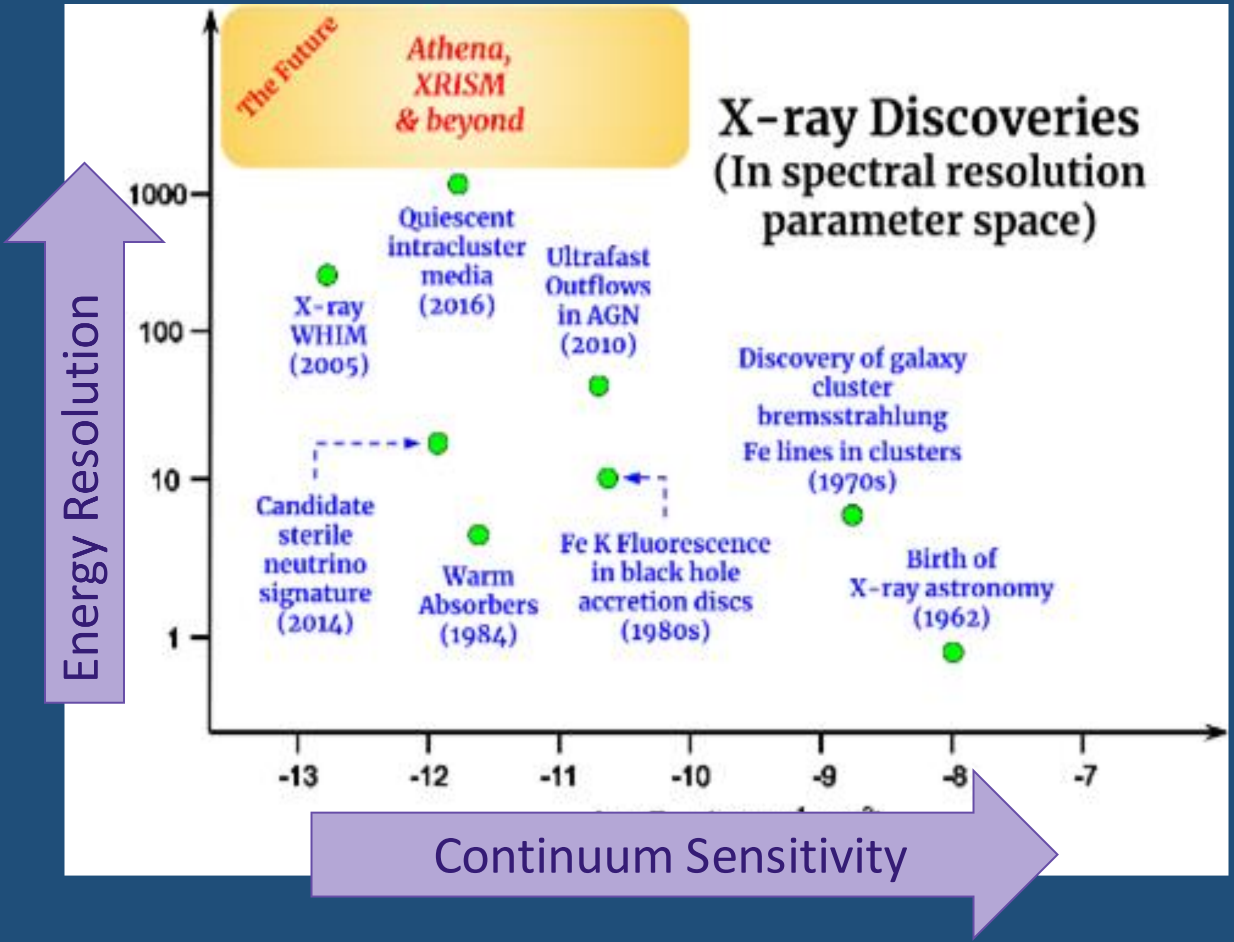
Andromeda Galaxy by JWST

X-ray emitting objects:

- Galaxy Clusters
- Black holes in AGN
- Supernova Remnants
- X-ray Binaries

10^6 K < T_e < 10^8 K

What does spectral resolution buy us?



Accretion physics at high X-ray spectral resolution: New frontiers and game-changing science. From: P. Gandhi et. al (2022)
x-axis = continuum sensitivity of X-ray detecting instrument

High-resolution X-ray Spectra

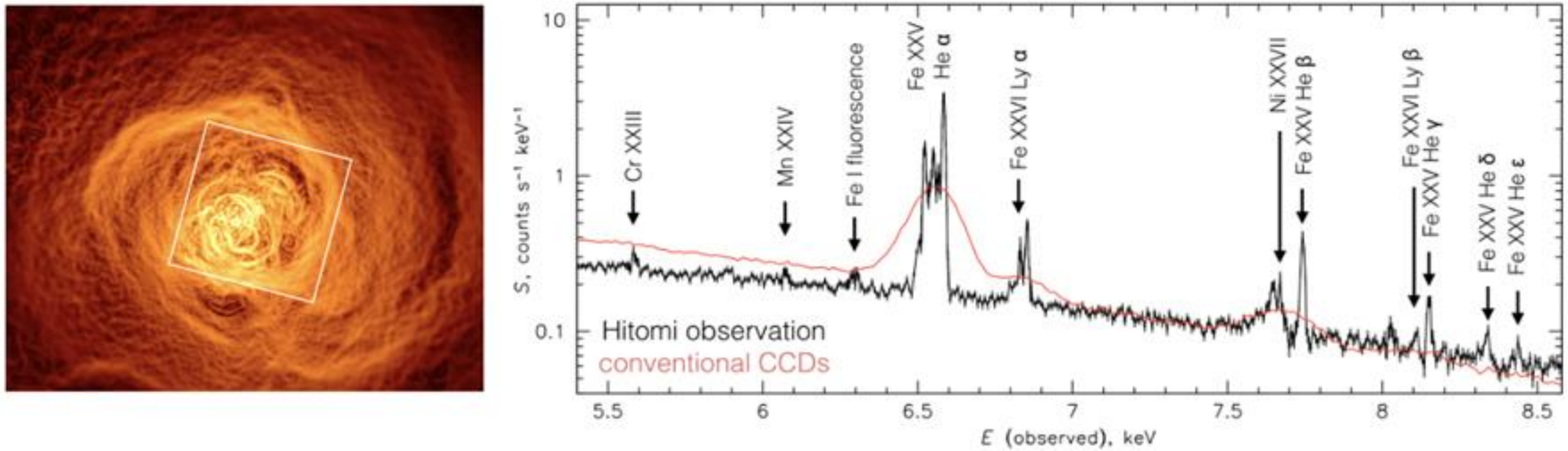


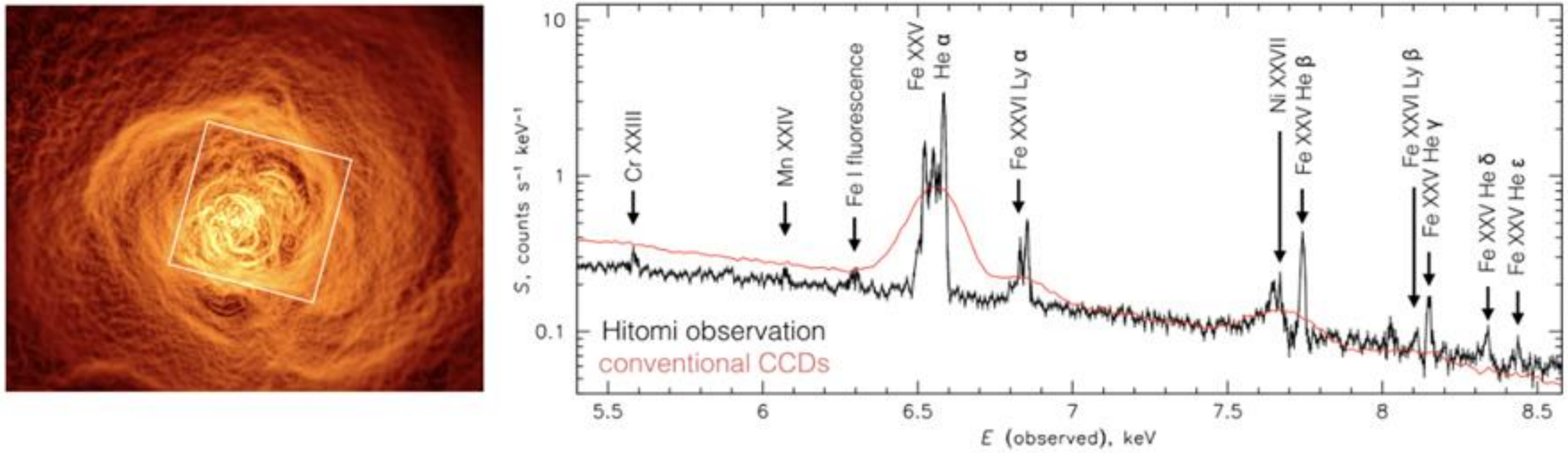
Figure 3: **Left:** *Chandra* X-ray image of the Perseus cluster core, filtered to emphasize structures in the hot gas[2]. **Right:** spectrum from the Perseus core (white square in the left panel) observed with *Hitomi's* microcalorimeter (black) and *Suzaku's* CCD imaging spectrometer (red). *XRISM* will provide similar high-resolution spectra in the 0.3 – 12 keV band for extended X-ray sources[3].

From: Science with XRISM
by XRISM science team

Hitomi X-ray Satellite
Launched 2016
JAXA

XRISM X-Ray Satellite
Launched 2023
JAXA-NASA

High-resolution X-ray Spectra



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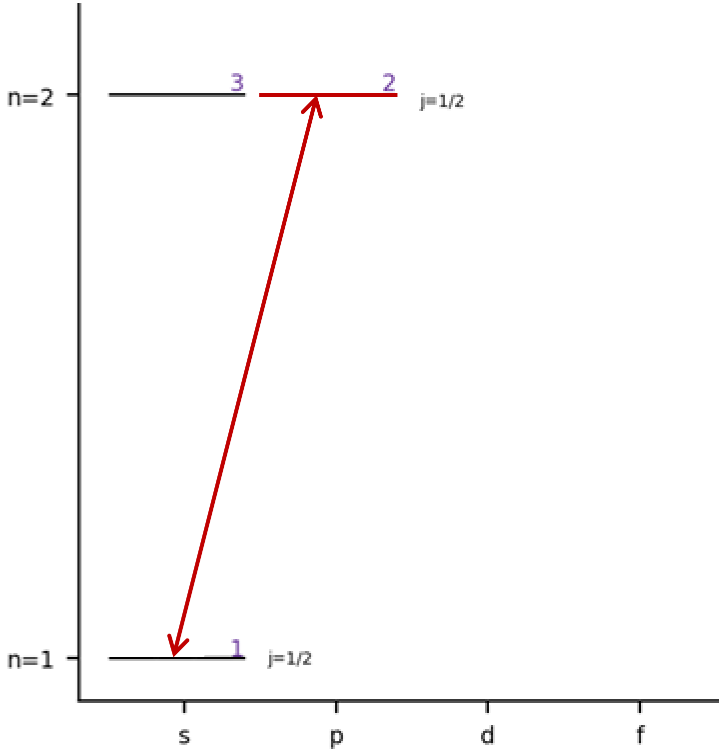

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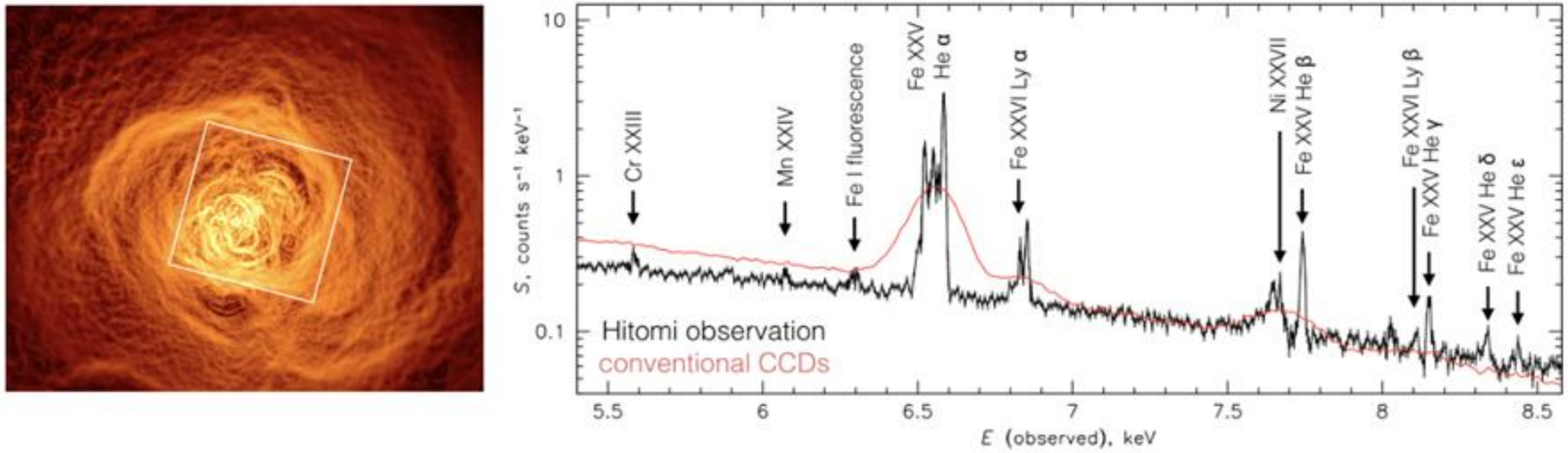
High-resolution X-ray Spectra



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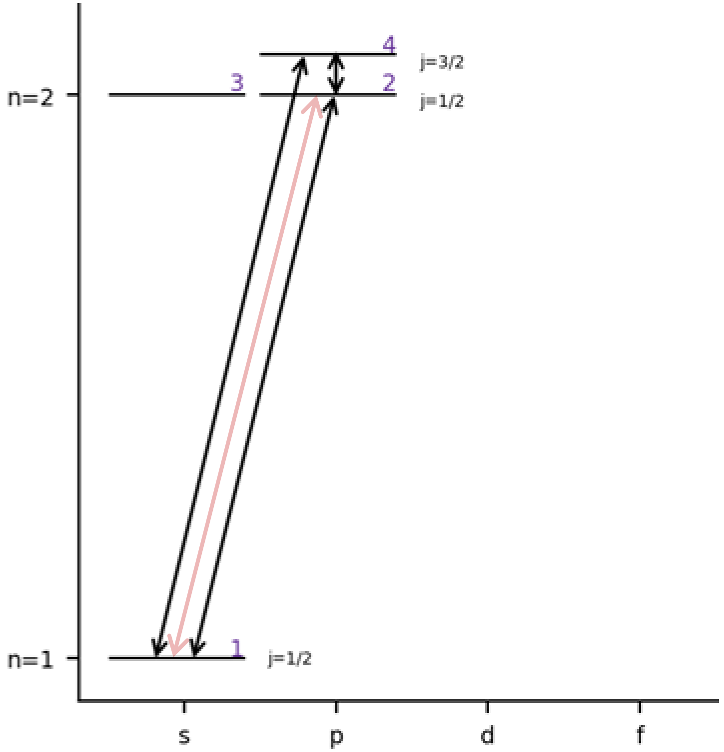

From: Science with XRISM
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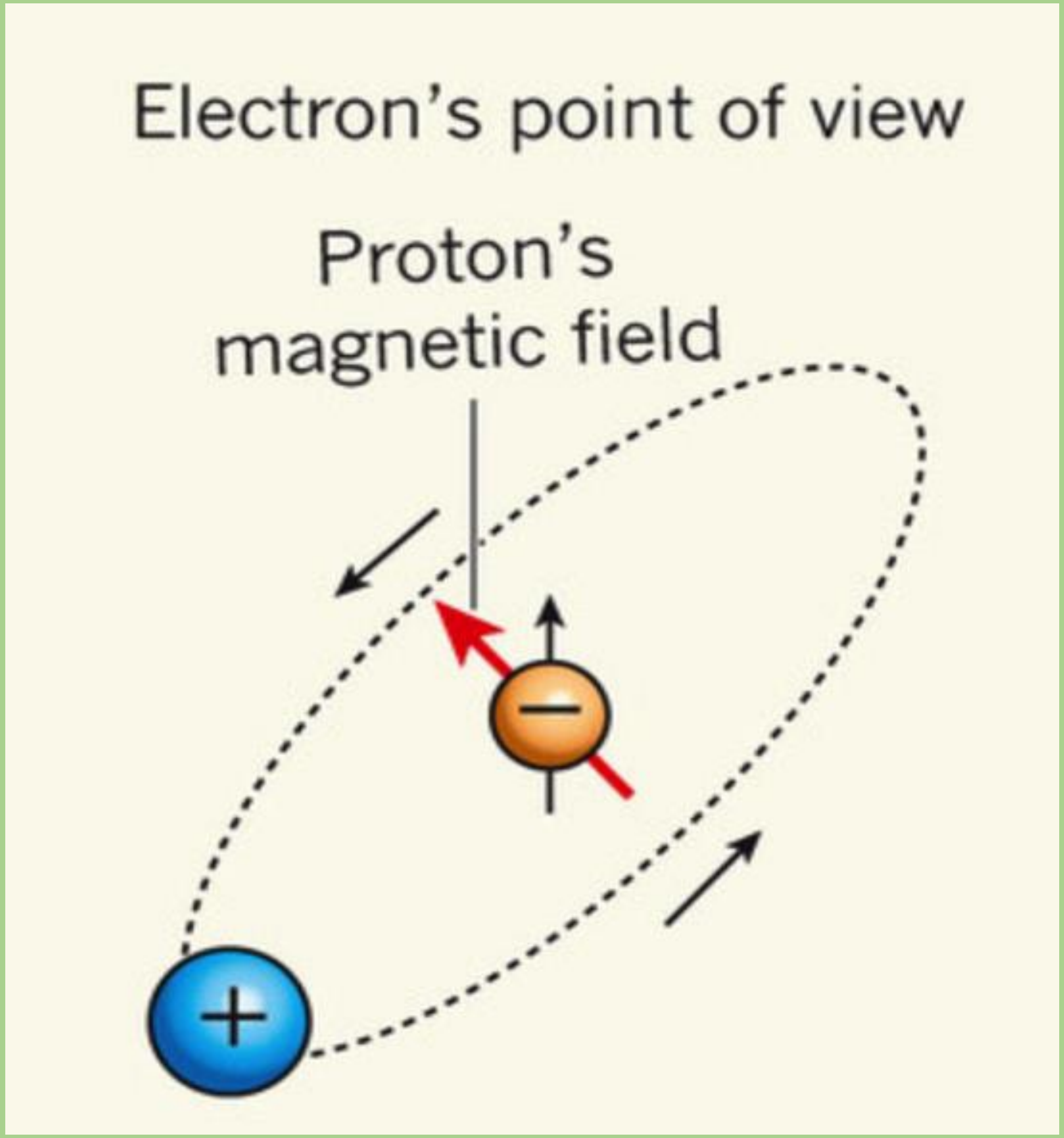
Fine-Structure Splitting: Quantum Theory



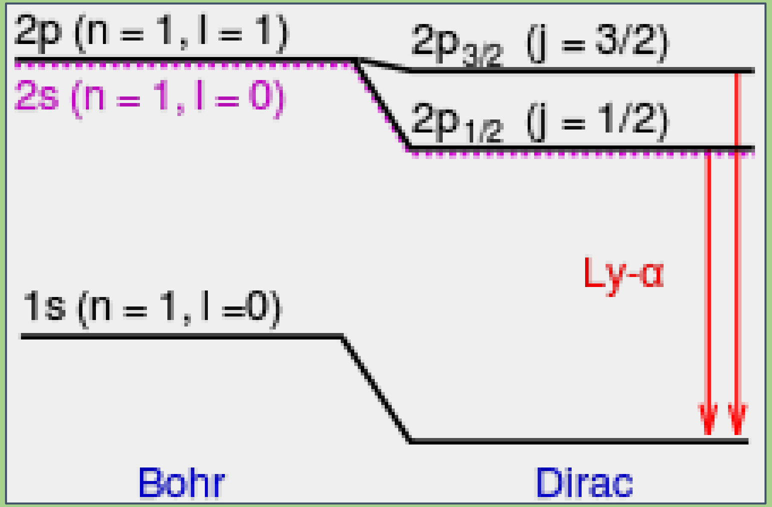
$$H = \mu_e . \mathbf{B}_N$$

$$\mathbf{B}_N \propto \mathbf{L}_e \qquad \mu_e = -\frac{e}{m}\mathbf{S}_e$$

Spin-Orbit Coupling $H \propto \mathbf{S}.\mathbf{L}$

$$E_n^0 + E_{nj}^{FS} = m_e c^2 \left[1 + \left(\frac{\alpha Z}{n - k + \sqrt{k^2 - \alpha^2 Z^2}} \right)^2 \right]^{-\frac{1}{2}} - m_e c^2$$

Fine structure splitting



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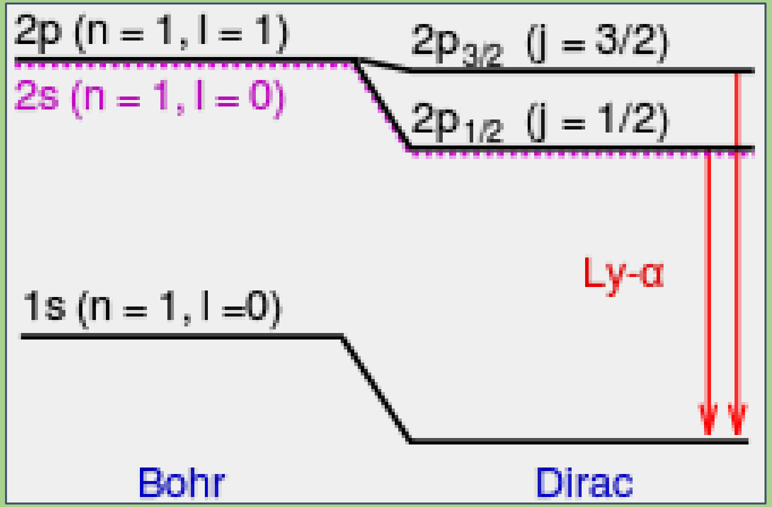
XRISM accuracy = 0.5 eV

Fine structure splitting



Fine-Structure Splitting: j-resolved Energy Levels

$$E_{n\mathrm{P}} = E_n^0 + E_{nj}^{FS} + E_{n,l=1,j}^{\mathrm{LS}} + E_{nj}^{M}$$

XRISM accuracy = 0.5 eV

Fine-Structure Splitting: j-resolved Energy Levels

$$E_{nP} = E_n^0 + E_{nj}^{FS} + E_{n,l=1,j}^{LS} + E_{nj}^{M}$$

Lamb Shift Correction:

$$E_{n,l>0,j}^{LS} = \frac{8Z^4\alpha^3}{3\pi n^3} Ry \left[\log \frac{Z^2 Ry}{K_0(n,l)} + \frac{3}{8}\frac{c_{lj}}{2l+1}\right]$$

$$c_{lj} = \begin{cases} (l+1)^{-1}, & \text{j=l+1/2,} \\ -l^{-1}, & \text{j=l-1/2.} \end{cases}$$

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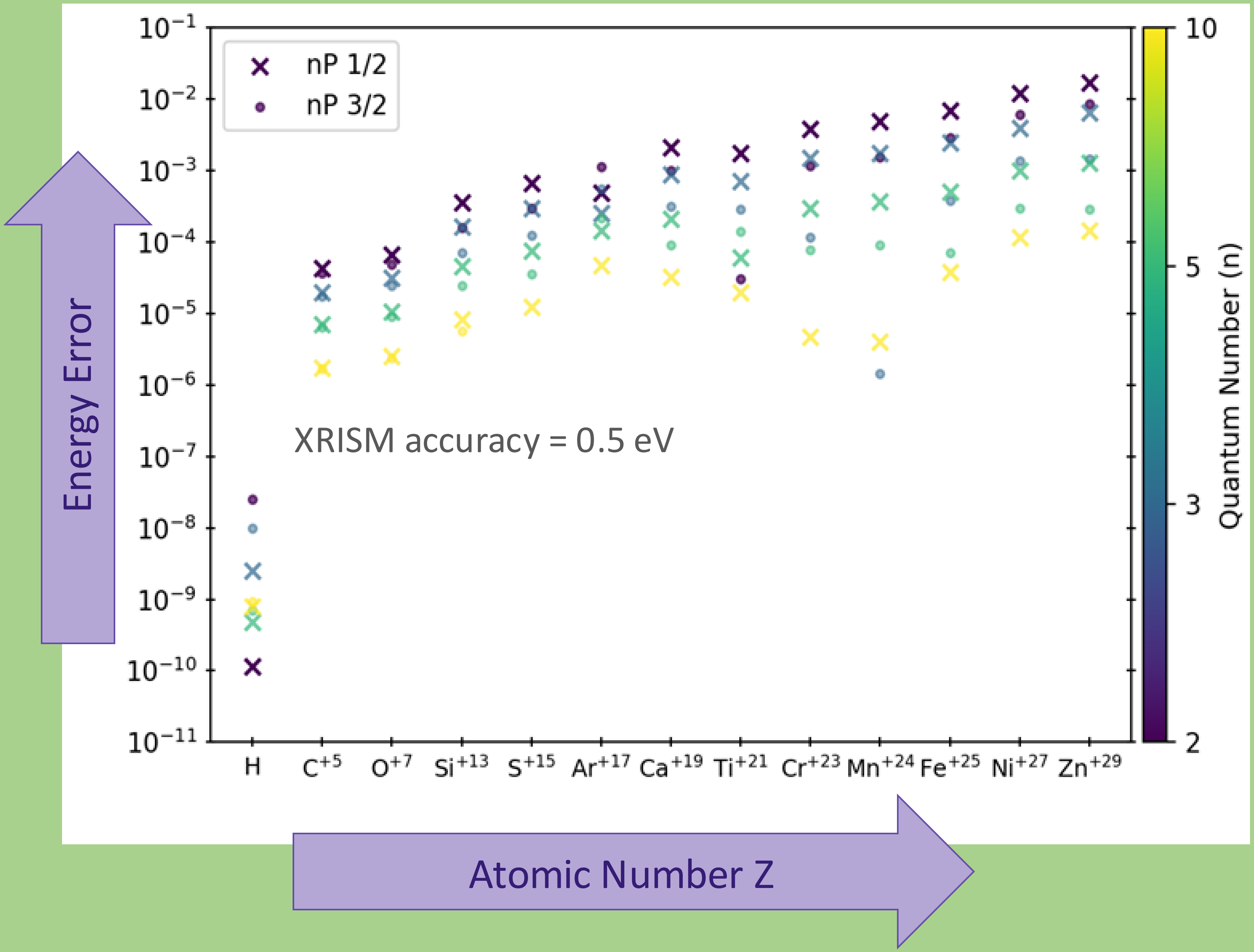
$$E_{nj}^{M} = m_e c^2 \frac{m_e}{m_N}\frac{(\alpha Z)^2}{2N^2} - \mu c^2 \left(\frac{m_e}{m_N}\right)\frac{(\alpha Z)^2}{2n^2}$$

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

where $k = j + 1/2$

Fine-Structure Splitting: j-resolved Energy Levels



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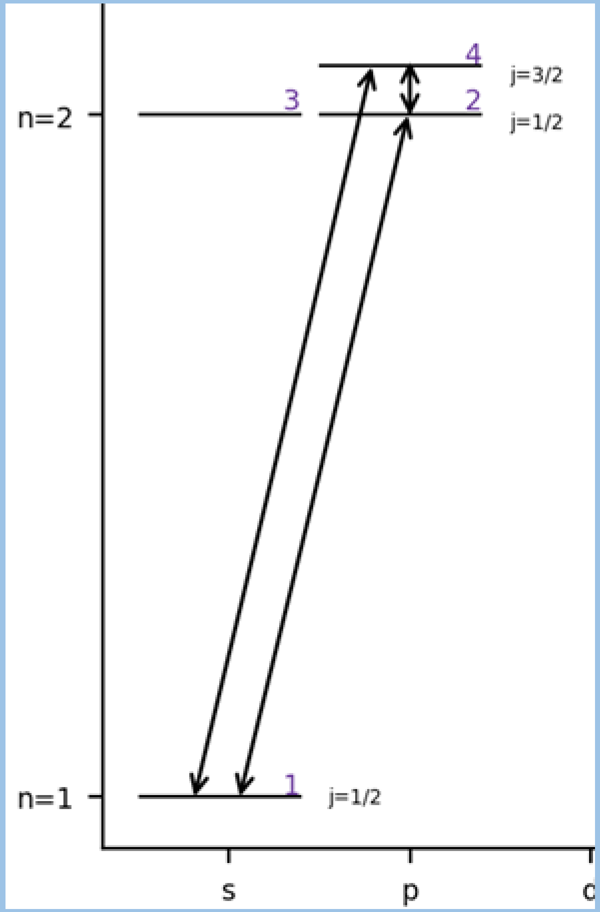
Fine-Structure Splitting: j-resolved Level Population Density



Radiative Transfer:

$$n_{2p} A_{21} \beta_{net} = \sum_j n_{2pj} A_{2pj} \beta_j$$

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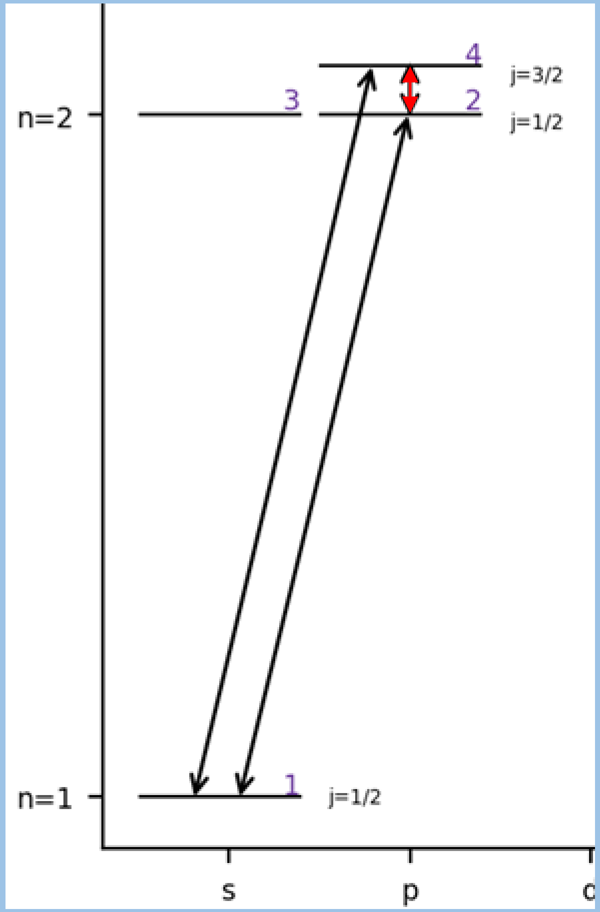

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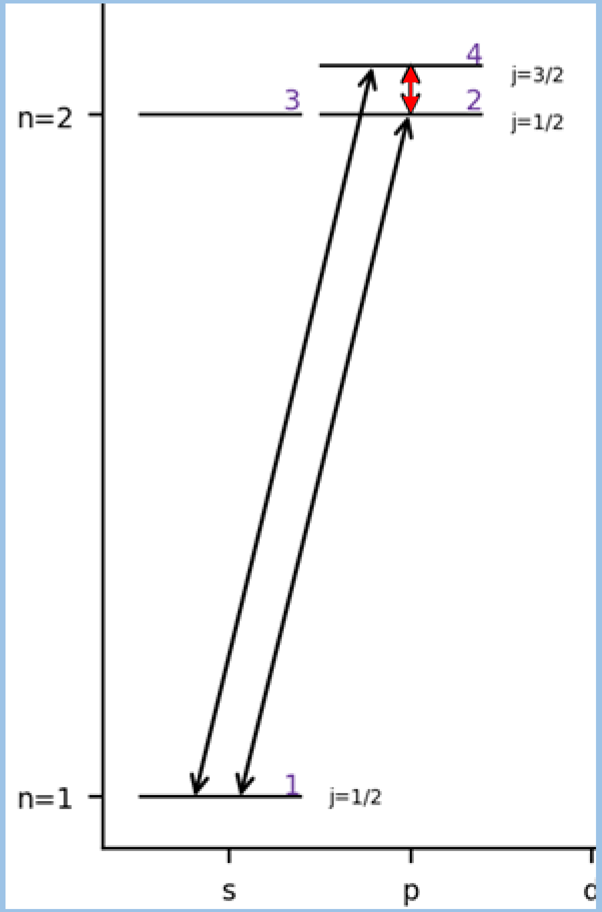

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Critical density:

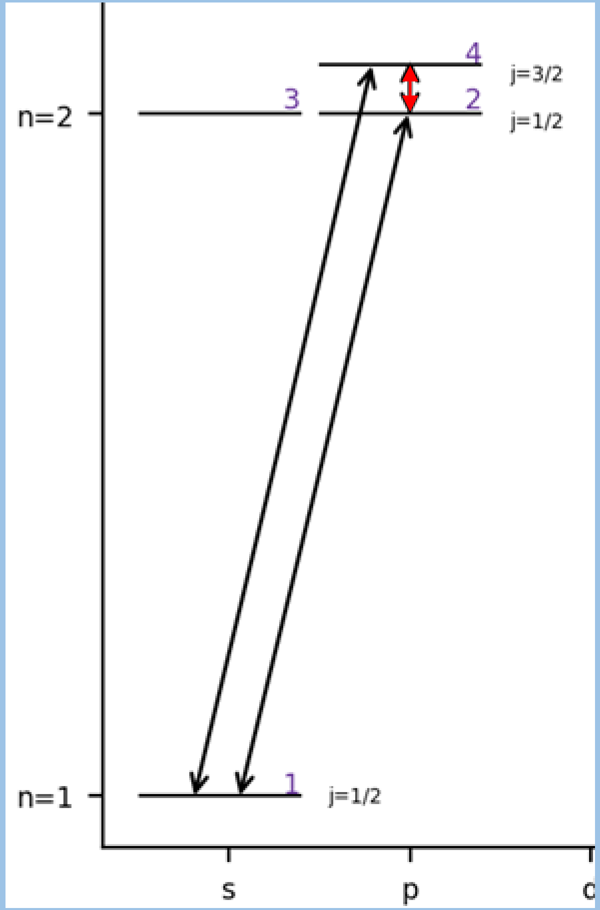
Collisional Deexcitations = Radiative Deexcitations

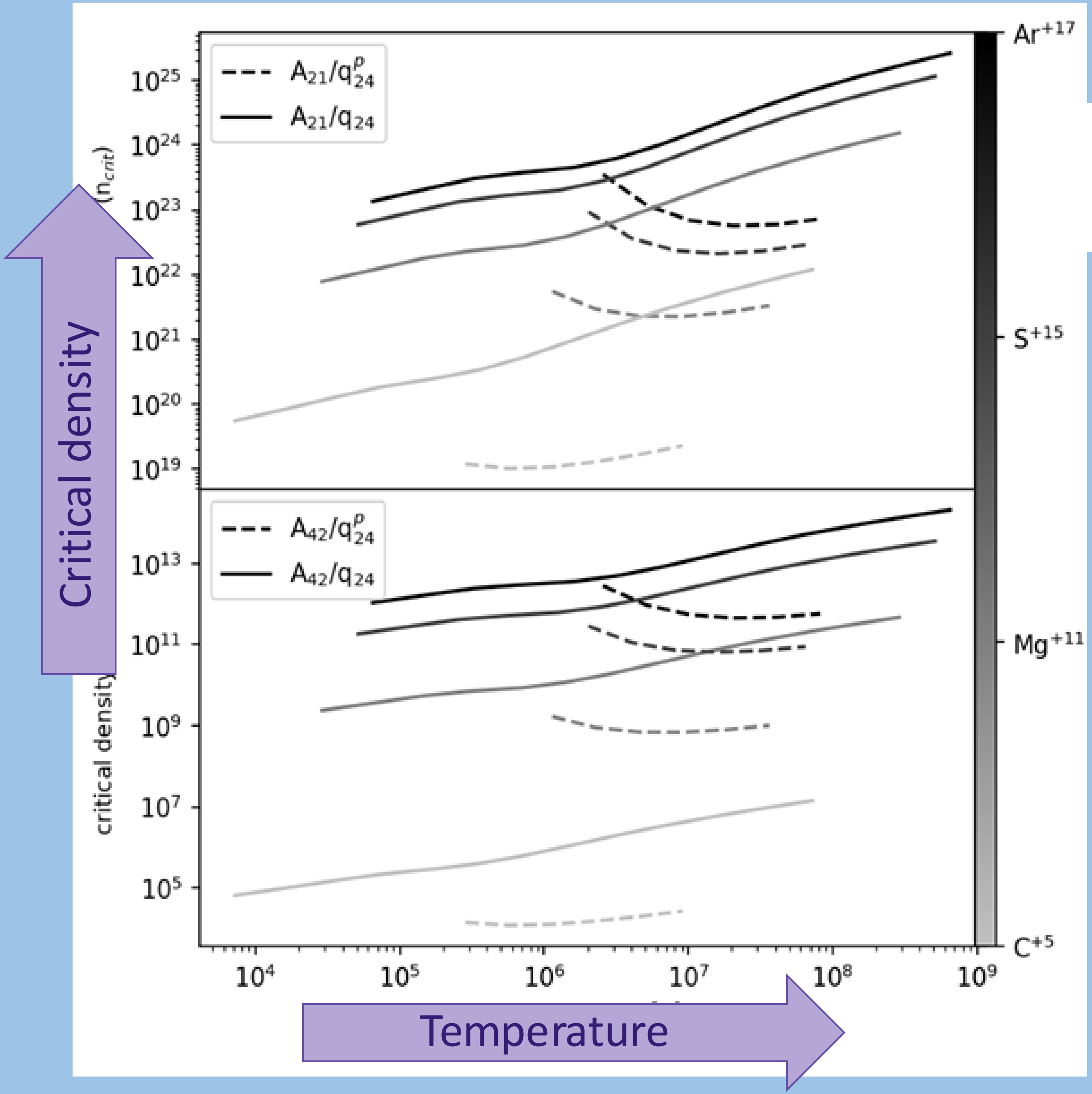
$$n_{\rm crit} = A_{\rm ul}/q_{\rm lu}$$

Low-density limit: $n_{gas} < n_{crit}$
Radiative > Collisions

High-density limit: $n_{gas} > n_{crit}$
Radiative < Collisions

Fine-Structure Splitting: j-resolved Level Population Density





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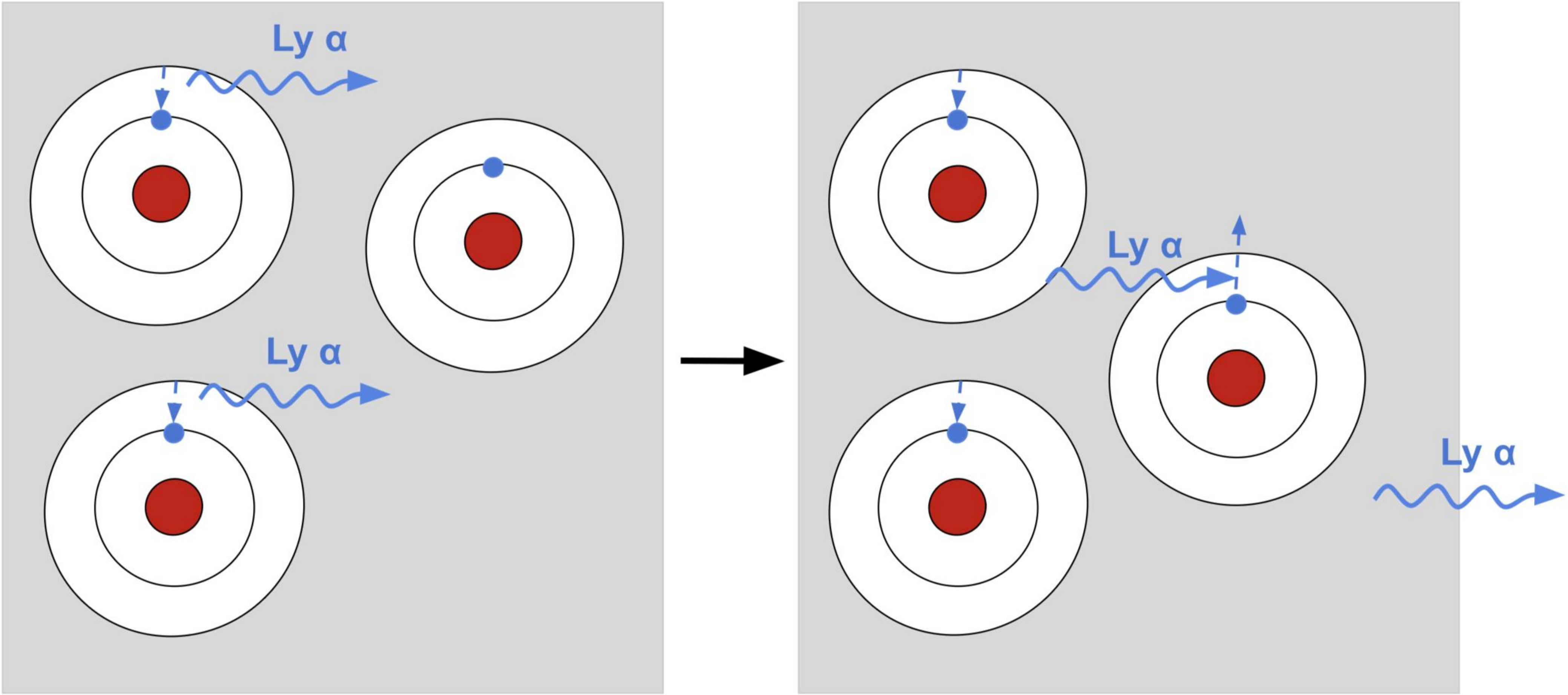
Simulating High-resolution X-rays: Radiative Transfer Effects

Radiative Trapping



Simulating High-resolution X-rays: Radiative Transfer Effects

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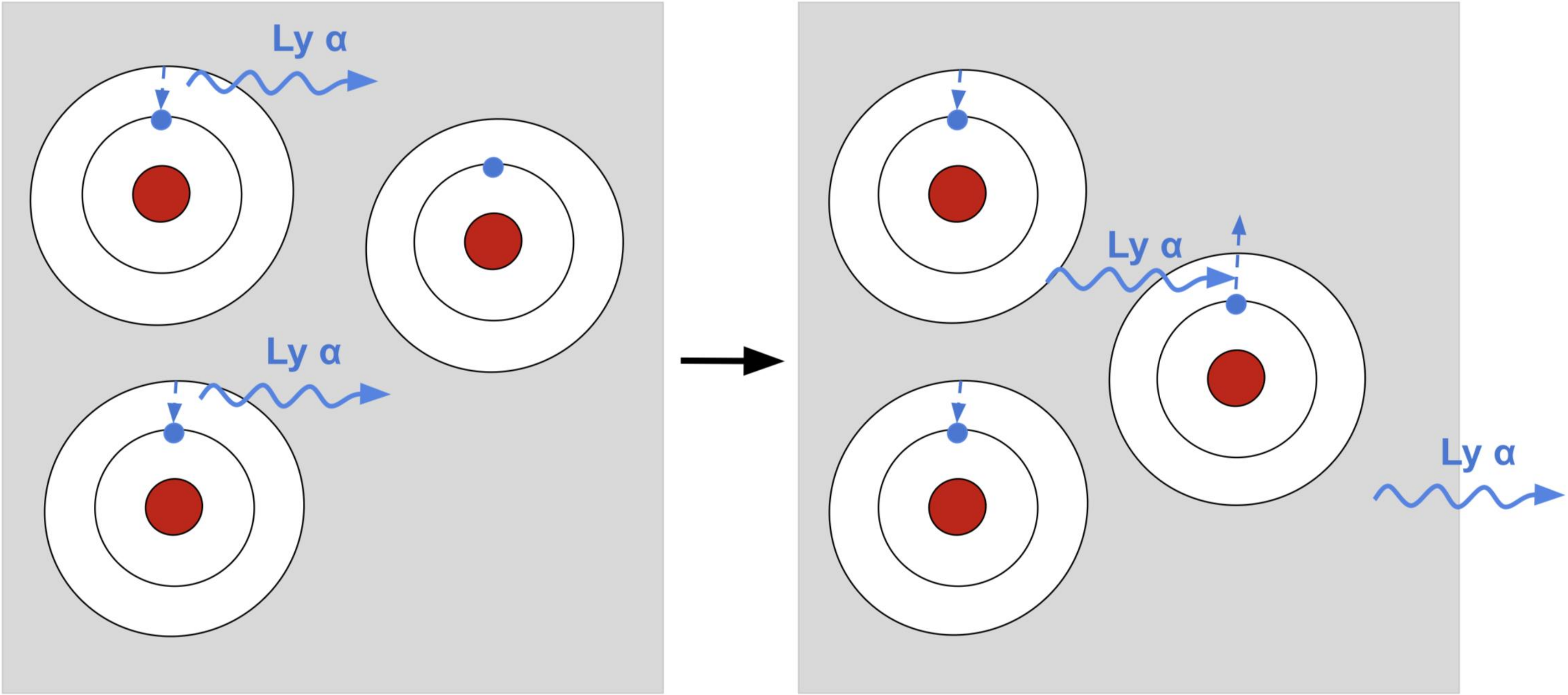
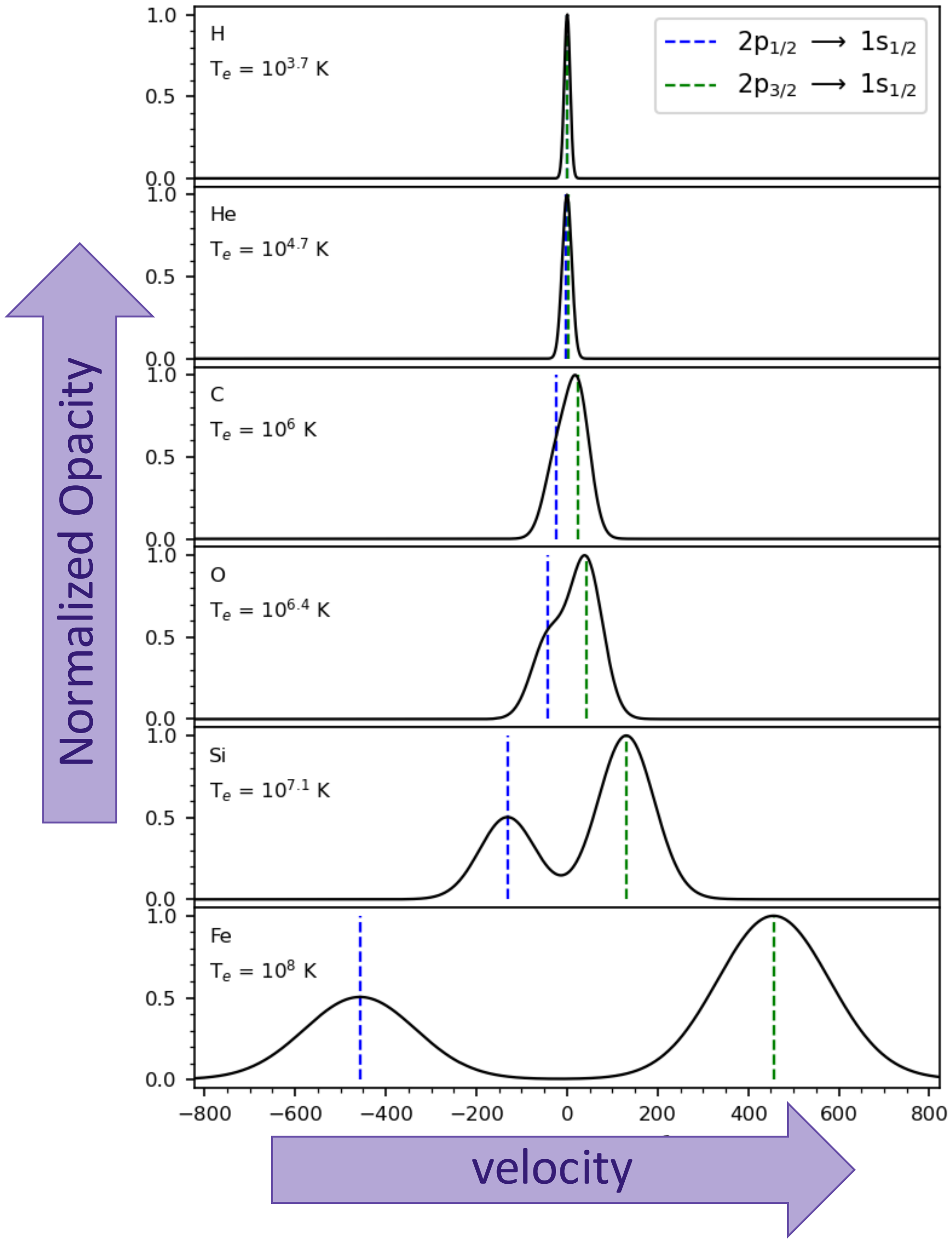


Escape Probability Approximation: $A_{ul} \rightarrow \beta A_{ul}$

Simulating High-resolution X-rays: Line



$$\beta \equiv k_c/k_L$$

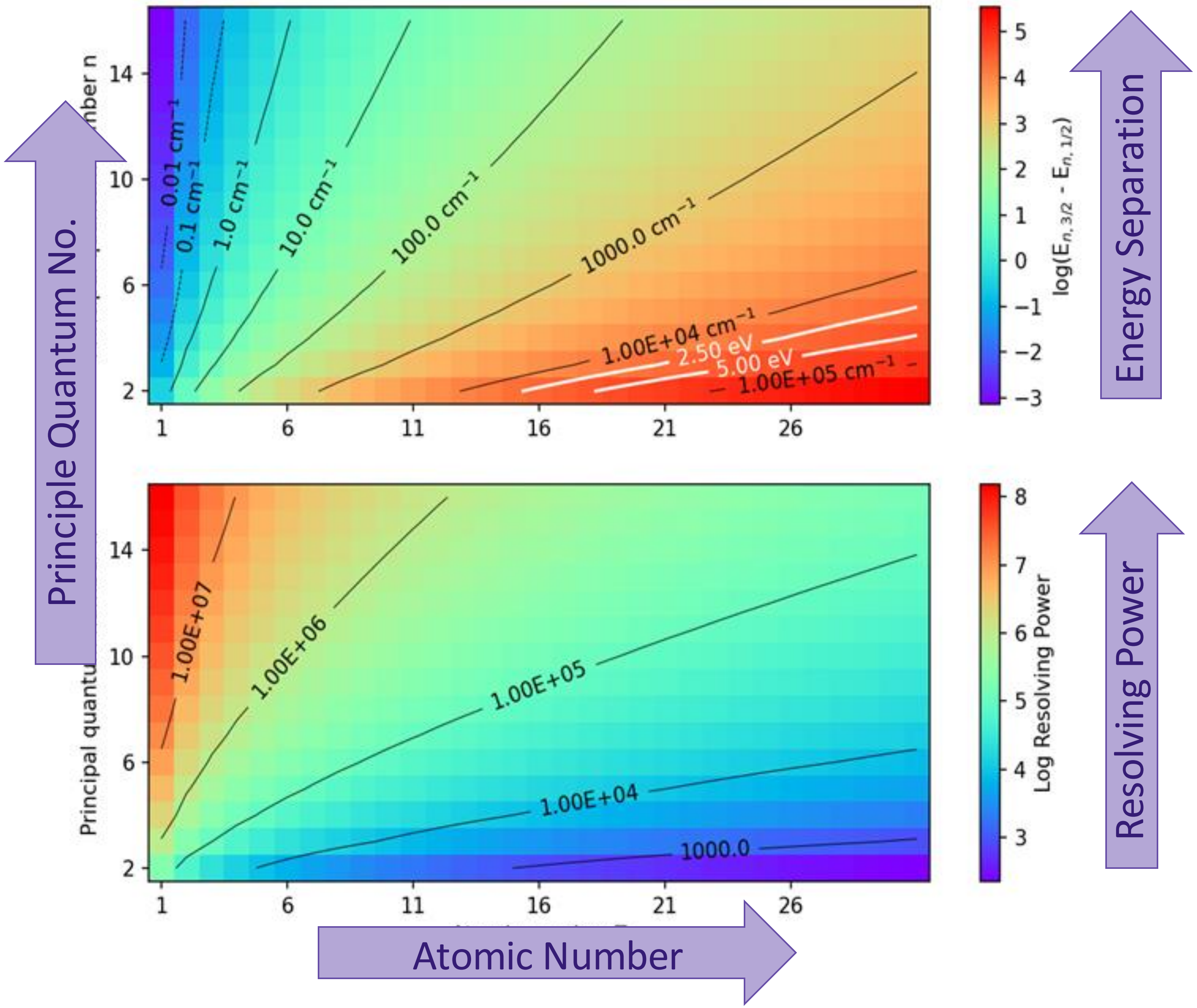
$$k_L = \frac{N_1 B_{12} h\nu_0}{4\pi\Delta}$$

$$k_L = N_1 \kappa_L \sqrt{\pi}/\Delta_v$$

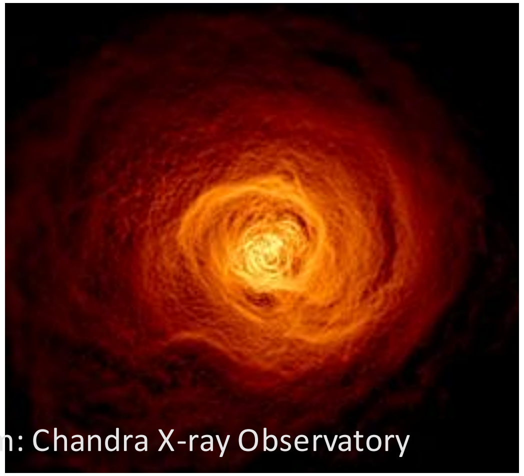
$$k(x) = k_L \frac{1}{\sqrt{\pi}} H(a,x) = \frac{N_1 \kappa_L}{\Delta_v} H(a,x)$$

$$k_L \approx k(0)\sqrt{\pi}$$

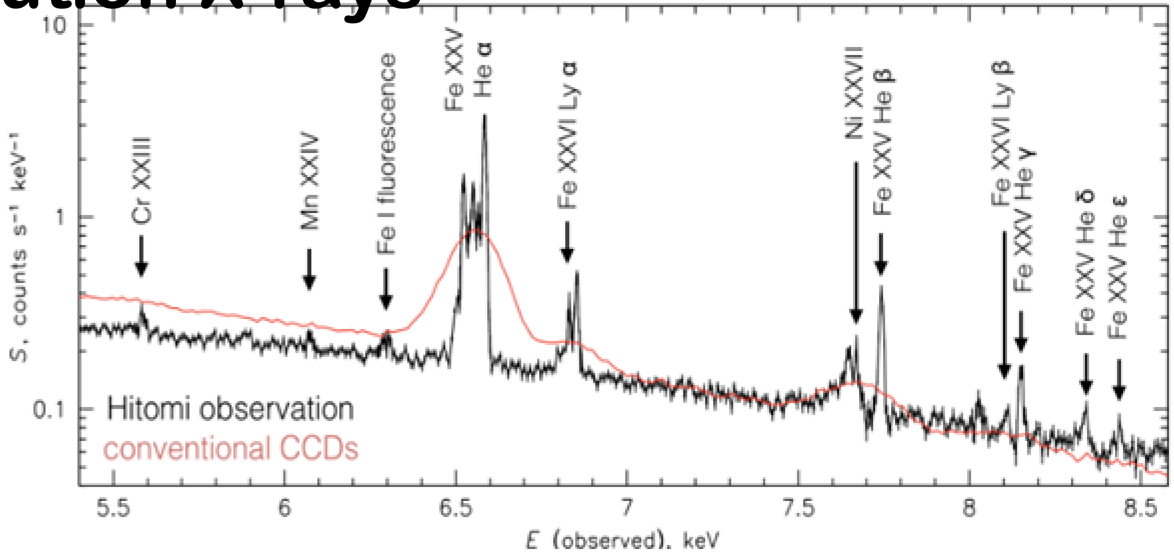
Simulating High-resolution X-rays

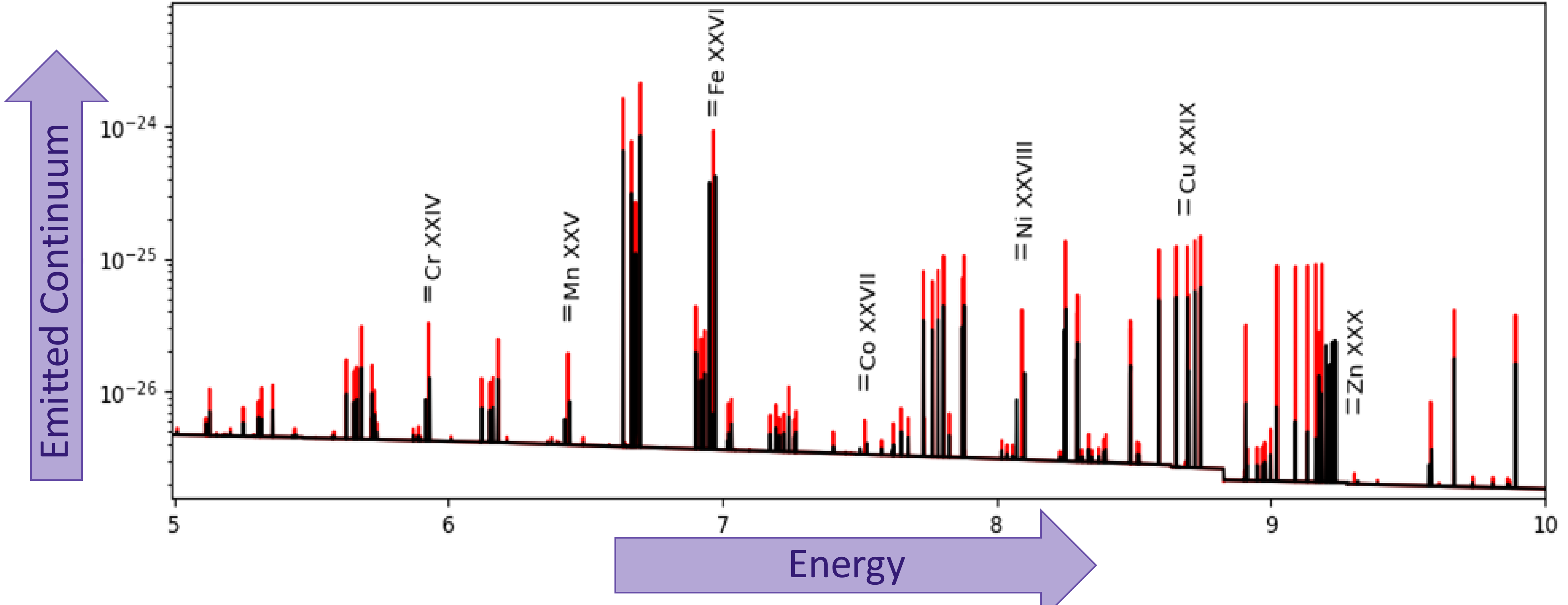


Simulating High-resolution X-rays



From: Chandra X-ray Observatory





Useful features

Hazy 1:

12.1.1 How many levels do we include?

Some models can include many hundreds to thousands of levels. The strongest lines tend to come from lower levels, although high levels can be quite important at high densities. Very large models, with the greatest number of levels, give the best spectroscopic accuracy but can take quite some time to compute. By default we include an intermediate number of levels, chosen as a compromise between execution time and an adequate model of the emission and cooling. The default number of resolved and collapsed levels can be found in LineLabels.out in the CLOUDY docs directory.

Useful features

>> cloudy/docs/LineLabels.txt

```
#index  label   wavelength      comment
0       zero                     0            # type: i, null placeholder
1       Unit                1.00000A          # type: i, unit integration placeholder
2       UntD                1.00000A          # type: i, unit integration placeholder
####    general properties.............................
3664    H  1 M1             1215.67A          # type: t, index=1, 2 Elow=0   H-like,   1^2S -   2^2S
3669    H  1                1215.67A          # type: t, index=1, 3 Elow=0   H-like,   1^2S -   2^2P
3674    H  1                1025.72A          # type: t, index=1, 5 Elow=0   H-like,   1^2S - n=  3
3679    H  1                972.537A          # type: t, index=1, 8 Elow=0   H-like,   1^2S - n=  4
```

>> cloudy/docs/LineLabels.out: number of levels in the atomic model

```
 Number of levels in ions treated by iso sequences.
 ISO    Element  hi-n(l-resolved) #(l-resolved)  n(collapsed)
 H-like   H        10               55             15
 H-like   He       10               55             15
 H-like   Li        5               15              2
 H-like   Be        5               15              2
 H-like   B         5               15              2
 H-like   C         5               15             15
 H-like   N         5               15             15
 H-like   Fe       10               55             15
```

Useful features

Hazy 1:

12.2.2 Species "name" levels=[10,all]

This option allows the number of levels used in modelling the species to be altered from the default value, within the bounds of the transition rate data available to CLOUDY. The command

```
species "O+" levels=10
```

runs a model with 10 levels for the O^+ ion, rather than the default value.

Using **=all** rather than a numeric argument requests the maximum available number of levels. The equal sign is part of the keyword and must be specified with no space between it and **all**.

>> cloudy/docs/LineLabels.out: number of levels in the atomic model

```
Number of levels in ions treated by iso sequences.
ISO    Element  hi-n(l-resolved) #(l-resolved)  n(collapsed)
H-like   H        10               55              15
H-like   He       10               55              15
H-like   Li        5               15               2
H-like   Be        5               15               2
H-like   B         5               15               2
H-like   C         5               15              15
H-like   N         5               15              15
```

Useful features

Fe K blends in the current Cloudy:

>> cloudy/data/blends.ini

```
## Fe XXVI 2s1/2 + 2p1/2
set blend 1.78337 quiet
"Fe26 M1"      1.78330A
"Fe26"      1.78344A
end
## Fe XXVI K alpha
set blend 1.77982 quiet
"Fe26"      1.77802A
"Fe26 M1"      1.78330A
"Fe26"      1.78344A
end
```

- Note: some old Fe K lines that used to be in cloudy have now been removed.
e.g. Fe K cold

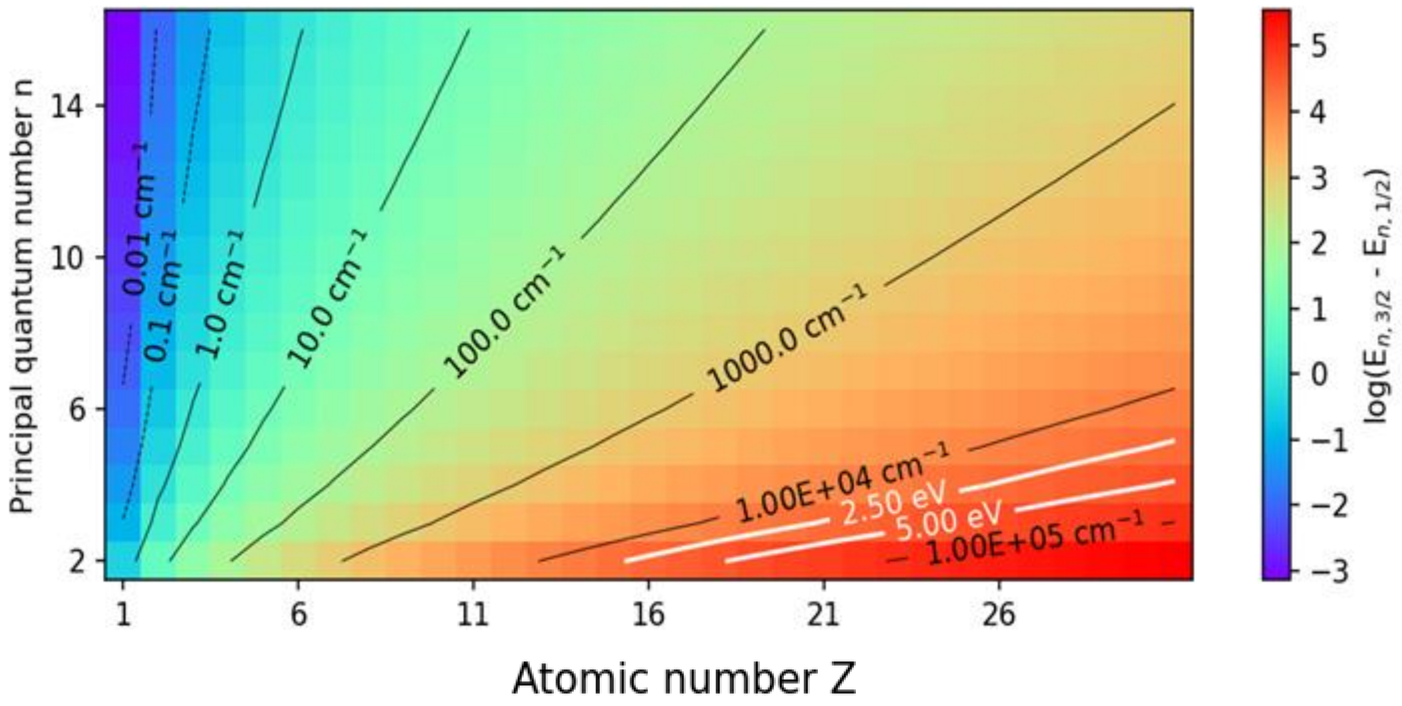
If you are interested please ask me!

Useful features

Database H-like Lyman extra resolution 0.25

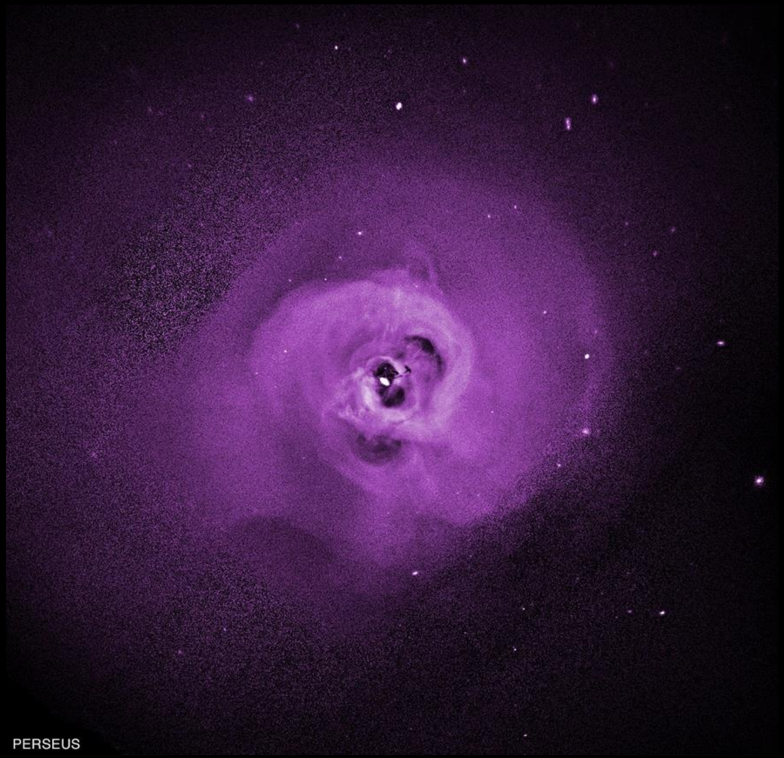
The nP to 1s lines of the H-like isoelectronic sequence are resolved into the fine-structure components. This commands determines down to which atomic species Z and upto which principle quantum number n the nP levels are resolved to nPj=1/2 and nPj=3/2 levels. The default resolution has been set to 1/10 in eV of the Athena high-resolution X-ray mission, 0.25eV.

This command does not affect the model atoms for H I and He II.



Some physics Cloudy can help us understand

```
set save preflix "Perseus_Ngrd"
constant temperature 4.7e7K
iterate
hden -1.5
metal solar 0.65 linear
stop column density 24 vary
grid 18 25 0.25
turbulence 150km/s
print line optical depths
print line column
print line sort wavelength
print line faint off -10
save grid ".grd" last no hash
save line list absolute ".lin" last no hash "linelist_fe_master.dat"
```




```
Fe26                 1.78344A    # j=3/2
Fe26                 1.77802A    # j=1/2
blnd             1.77982A # Fe26 Ka blend
blnd             1.50273A # Fe26 Kb blend
Si14             6.18584A # Si14 Ka1
Si14             6.18043A # Si14 Ka2
blnd             6.18222A # Si14 Ka blend
blnd             5.21719A # Si14 Kb blend
```

Some physics Cloudy can help us understand

```
set save prefix "Perseus_Ngrd"
constant temperature 4.7e7K
iterate
hden -1.5
metal solar 0.65 linear
stop column density 24 vary
grid 18 25 0.25
turbulence 150km/s
print line optical depths
print line column
print line sort wavelength
print line faint off -10
save grid ".grd" last no hash
save line list absolute ".lin" last no hash "linelist_fe_master.dat"
```

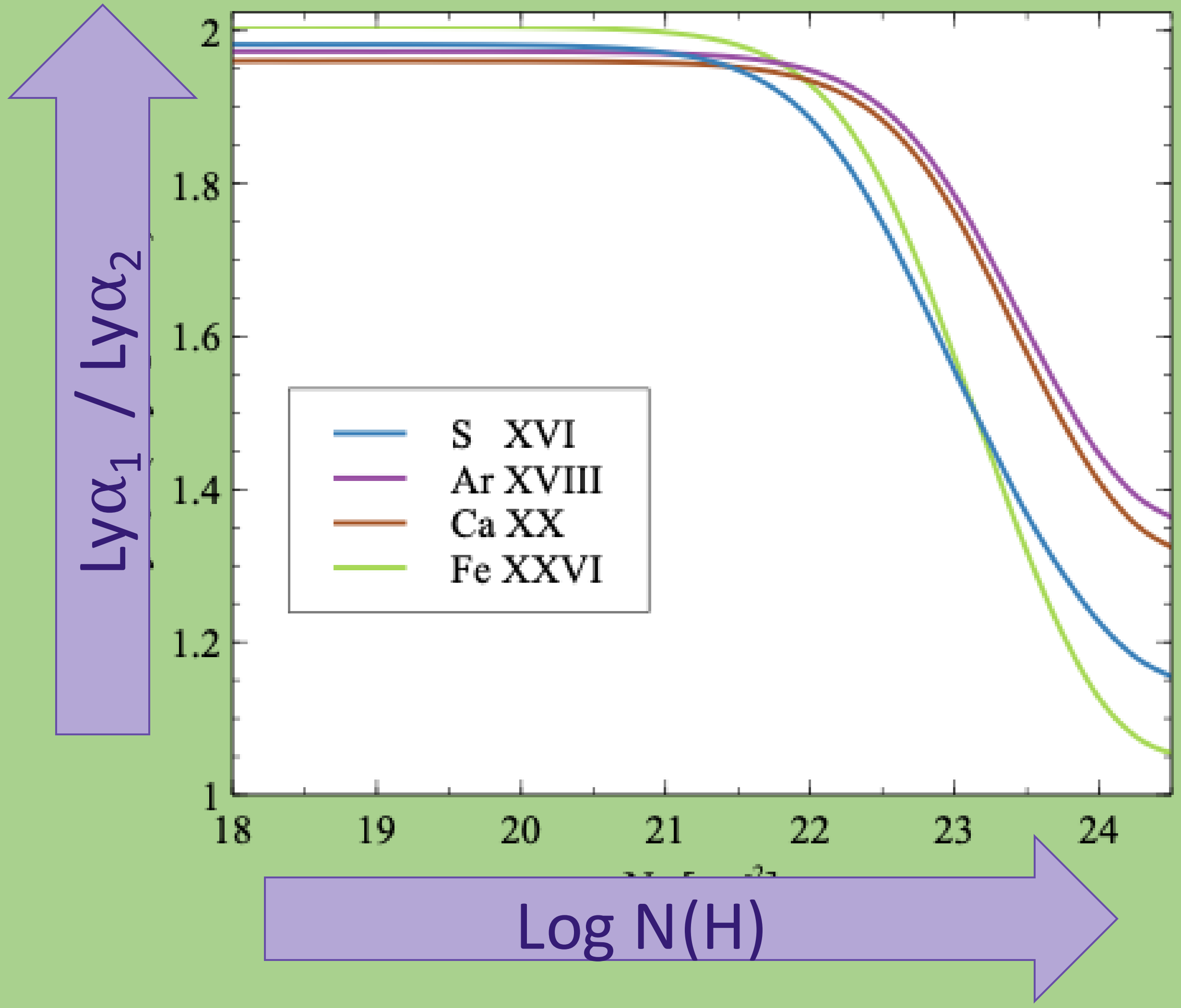
Perseus_Ngrid.grd

#Index	Failure?	Warnings?	Exit code	#rank	#seq	STOP COLU	grid parameter string
000000000	F	F	ok	6	0	18.000000	18.000000
000000001	F	F	ok	7	0	18.250000	18.250000
000000002	F	F	ok	8	1	18.500000	18.500000
000000003	F	F	ok	10	0	18.750000	18.750000

Perseus_Ngrid.lin

#lineslist	Fe26 1.78344A	Fe26 1.77802A	blnd 1.77982A	blnd 1.50273A
iteration 2	7.8612e-10	1.5770e-09	2.3941e-09	2.4615e-10
iteration 2	1.3979e-09	2.8044e-09	4.2575e-09	4.3772e-10
iteration 2	2.4860e-09	4.9870e-09	7.5711e-09	7.7838e-10
iteration 2	4.4208e-09	8.8684e-09	1.3464e-08	1.3842e-09

Column Density Indicators



Eddington Barbier approximation:

emergent line flux is determined by the source function at the location where line optical depth reaches 2/3 when integrated from observers point of view.