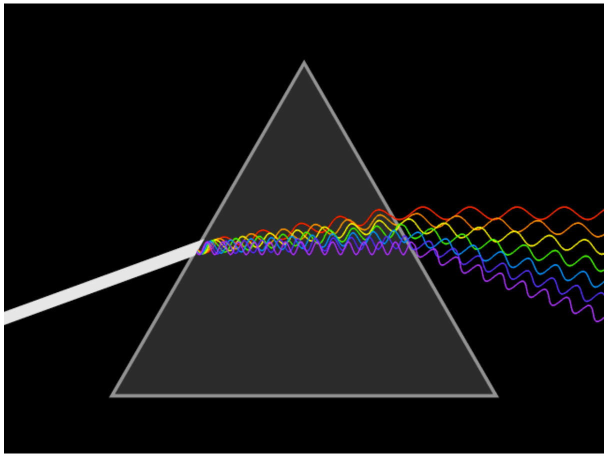
Data Analysis IV: X-ray Spectroscopy

- Three "dimensions" of (X-ray) Astronomy: Imaging, Timing, Spectroscopy

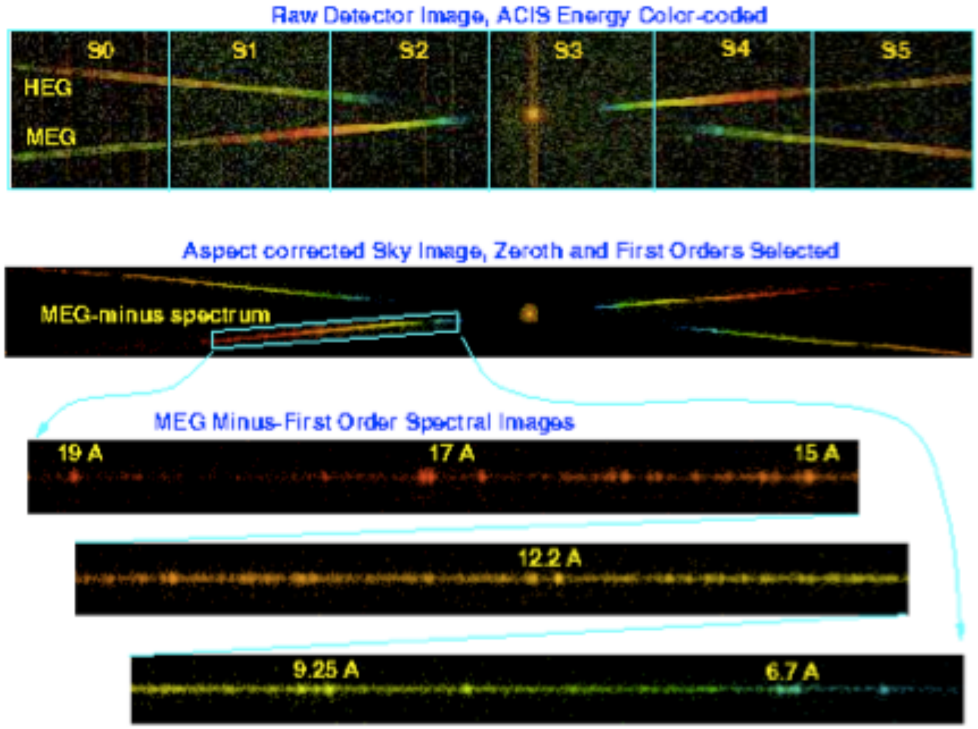
- Key factors in spectroscopy: throughput ("effective area"), bandpass, resolution $R=\lambda/\Delta\lambda$,

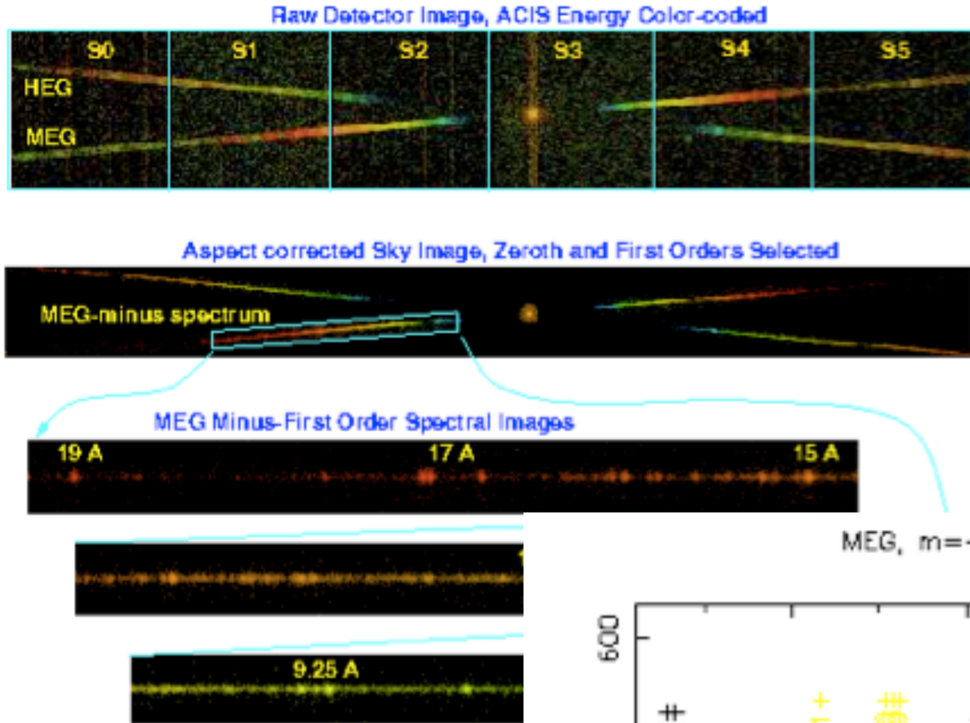
- Spectroscopy traditionally is dispersive, utilizing crystal and grating spectrometers (photons are waves)



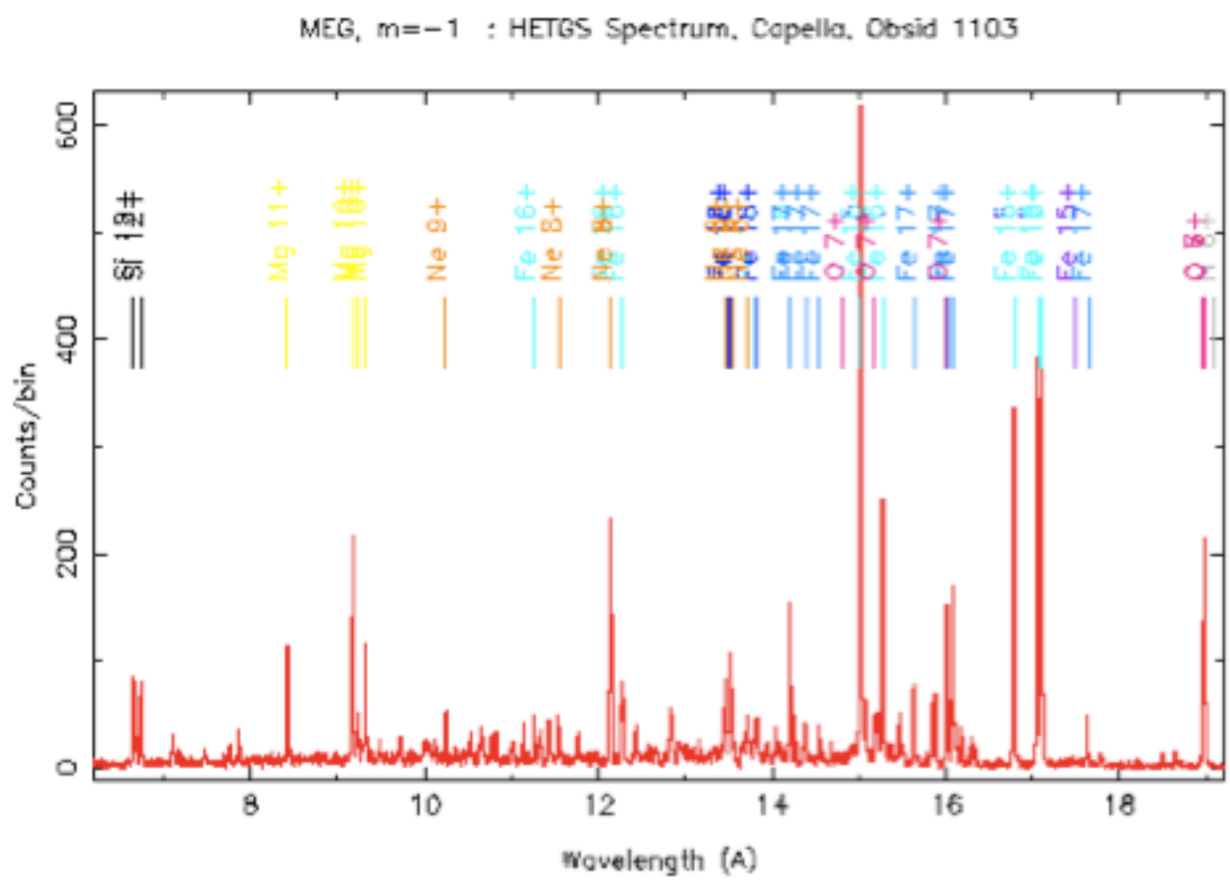
Currently operating X-ray grating spectrometers: *Chandra* HETG and LETG, *XMM-Newton* RGS

- Nondispersive spectrometers measure the energy (e.g., in the form of ionization or heat) deposited by X-rays (photons are particles)

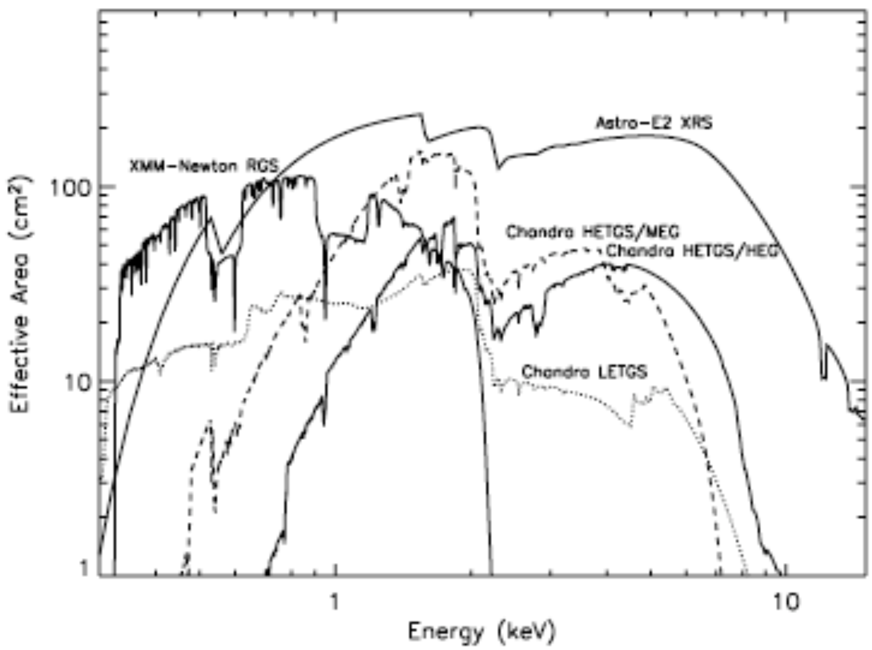

Raw Detector Image, ACIS Energy Color-coded
S0
S1
S2
S3
S4
S5
HEG
MEG
Aspect corrected Sky Image, Zeroth and First Orders Selected
MEG-minus spectrum
MEG Minus-First Order Spectral Images
19 A
17 A
15 A
12.2 A
9.25 A
6.7 A

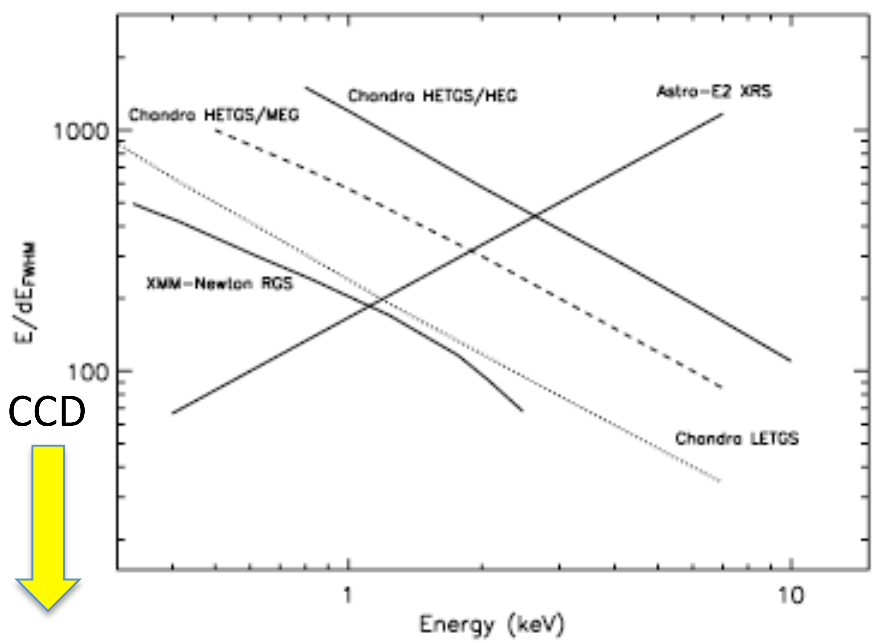


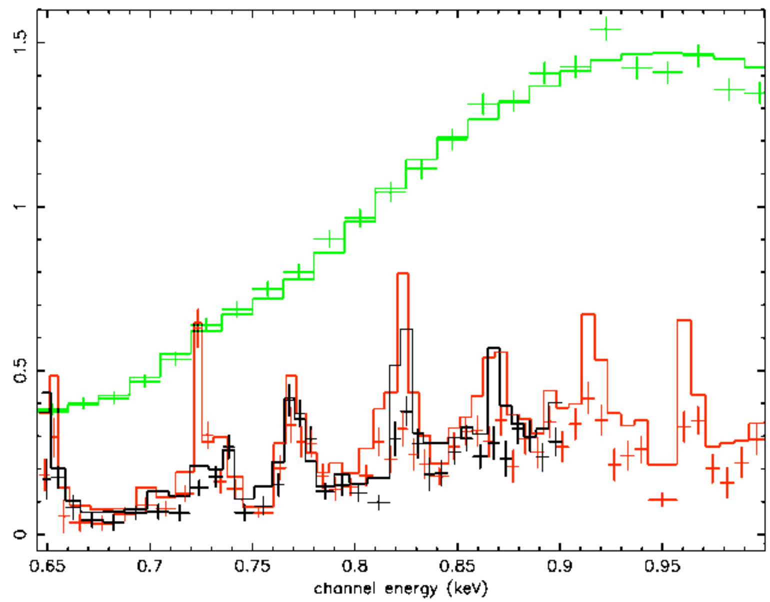
$R=\lambda/\Delta\lambda\approx1000$



High Resolution X-ray Spectroscopy: dynamics from line widths and shapes; physical conditions from line strengths and ratios





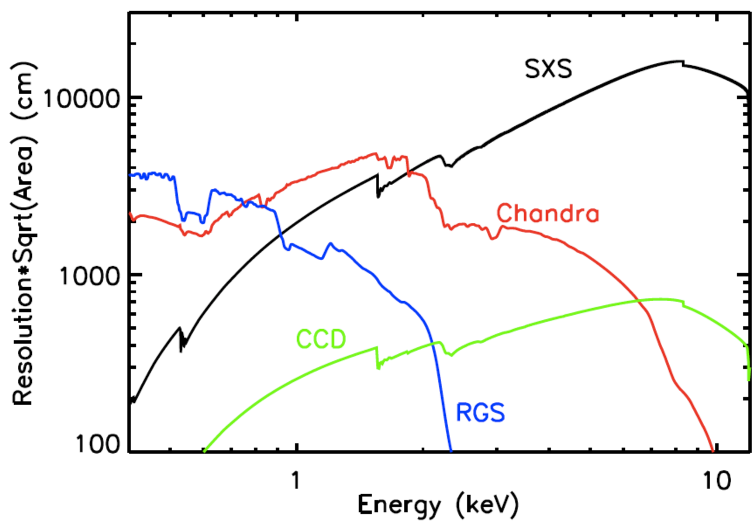


NGC 4472 Elliptical Galaxy Hot ISM:
XMM-Newton MOS CCD vs. RGS

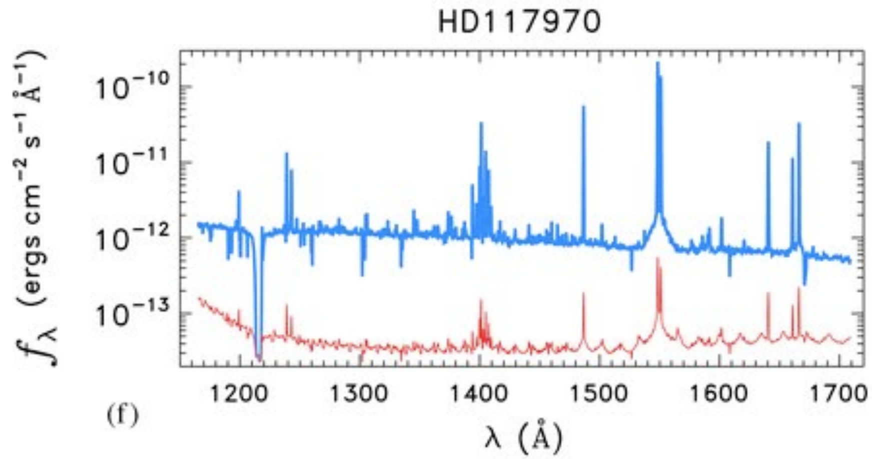
Dispersive X-ray spectrometers are most useful for point sources at E<2 keV.

"Medium" resolution X-ray CCD spectrometers are used to derive physical conditions and identify emission mechanism, and are pixelated.

The *Astro-H* SXS (launch: 2013) is a high resolution, pixelated, nondispersive X-ray spectrometer.



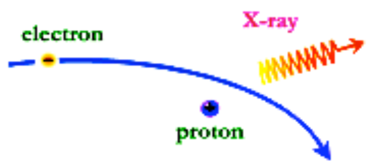
HST/STIS: $R=\lambda/\Delta\lambda \approx 100{,}000$



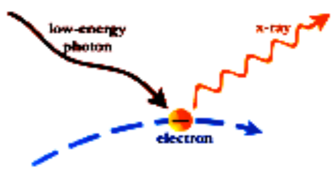
high energy particles → high energy photons

Some *X*-Ray Processes

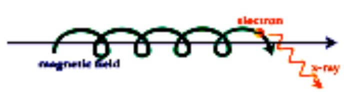
- Thermal Bremsstrahlung



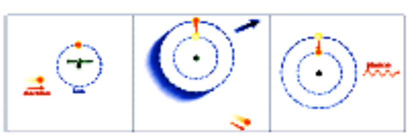
- Inverse Compton Scattering



- Synchrotron Radiation

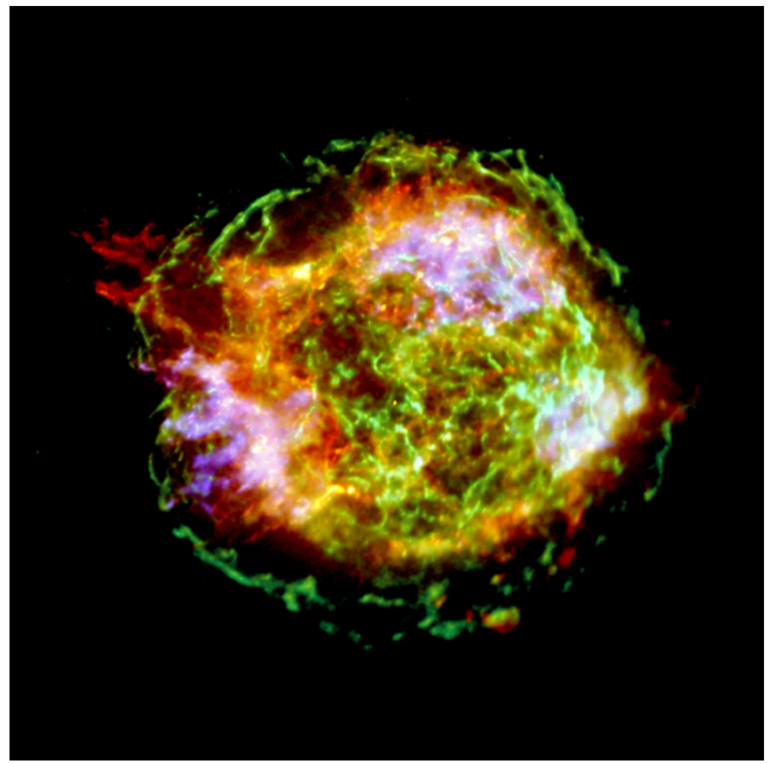


- Atomic Emission



Some X-ray Sources

- Supernova remnant, and γ-ray burst, shock waves



Cassiopeia A SNR

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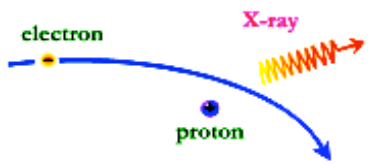

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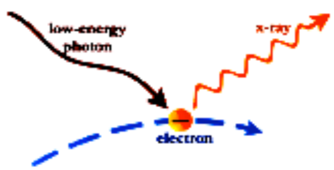

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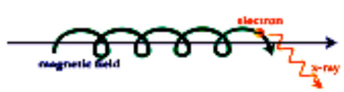

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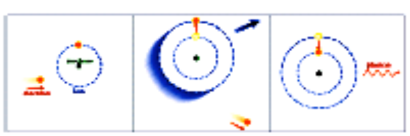

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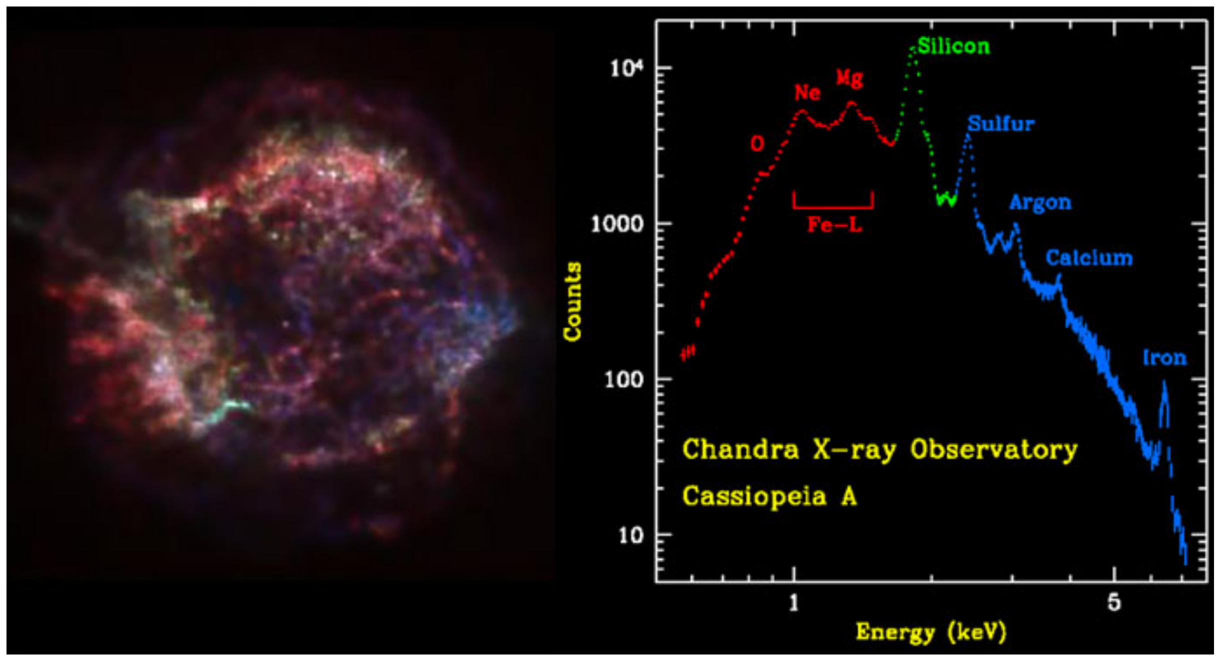

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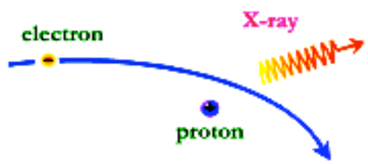

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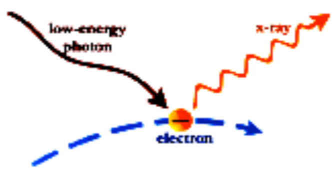

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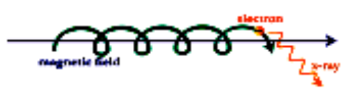

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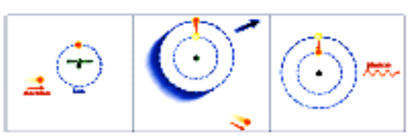
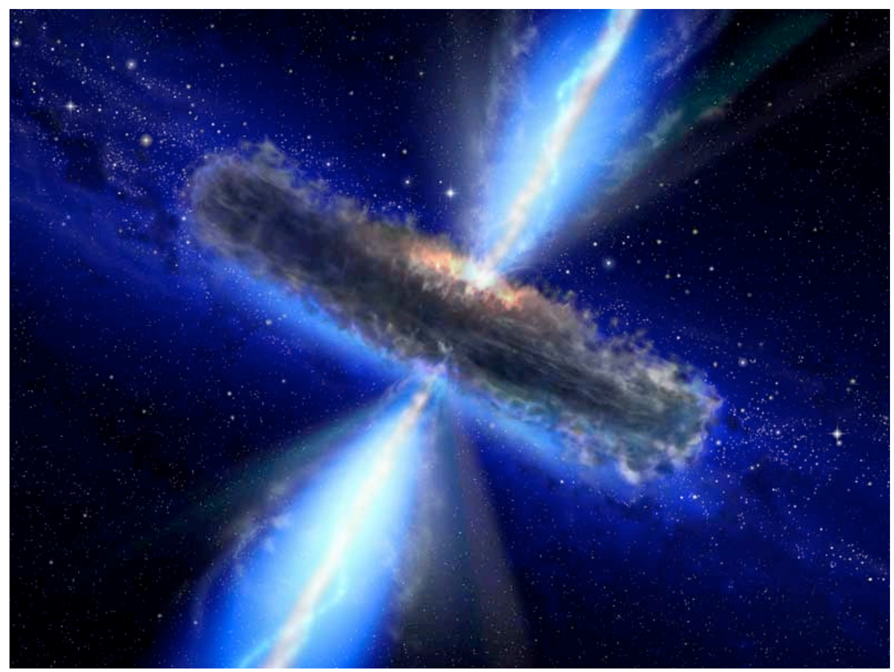


Some X-ray Sources

- Neutron star and (stellar and supermassive) black hole accretion disks and jets



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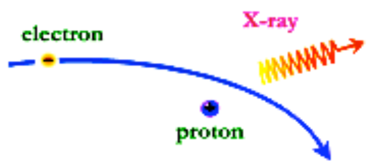

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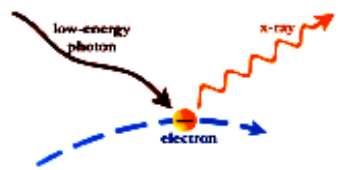

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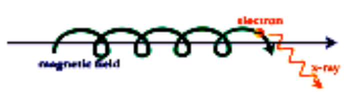

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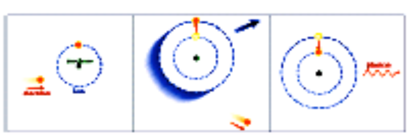

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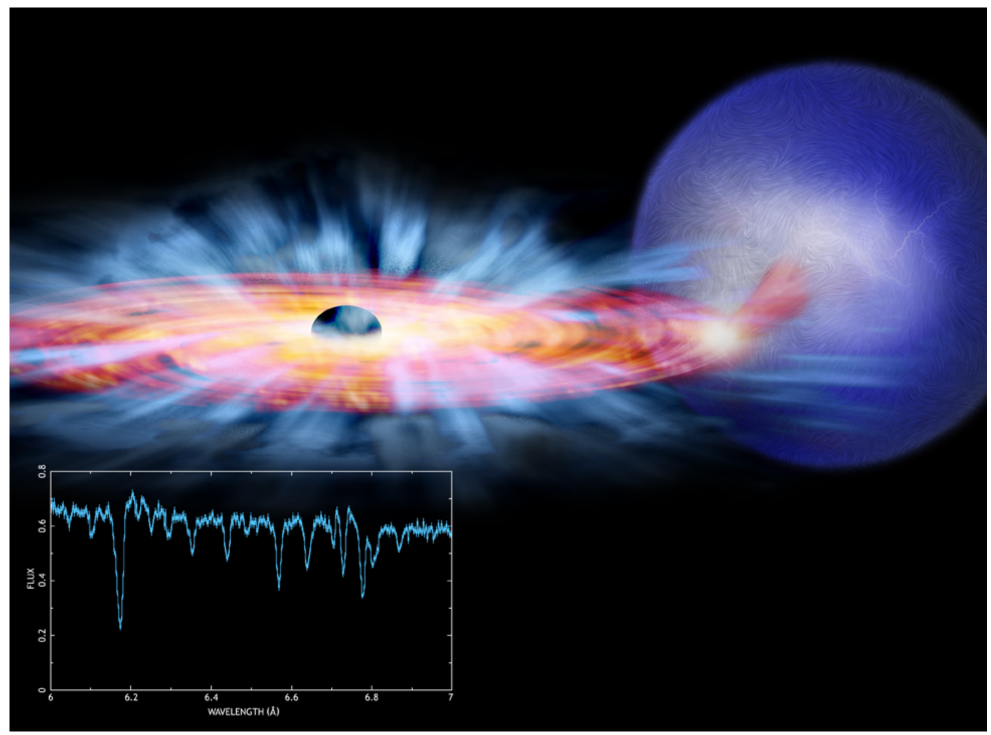
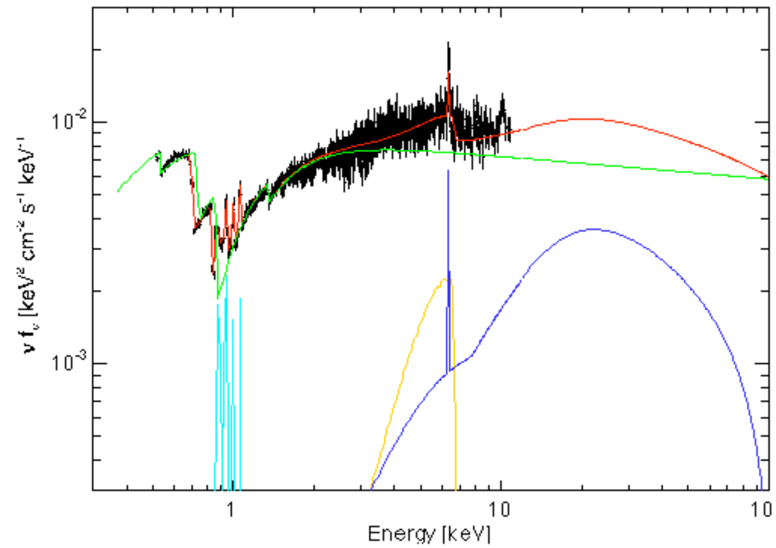


The Seyfert Galaxy MCG 6-30-15

Direct power-law from corona
“Reflected” component from Compton scattering off the accretion disk
A broad Fe fluorescent line from the disk near a spinnning superrmassive black hole



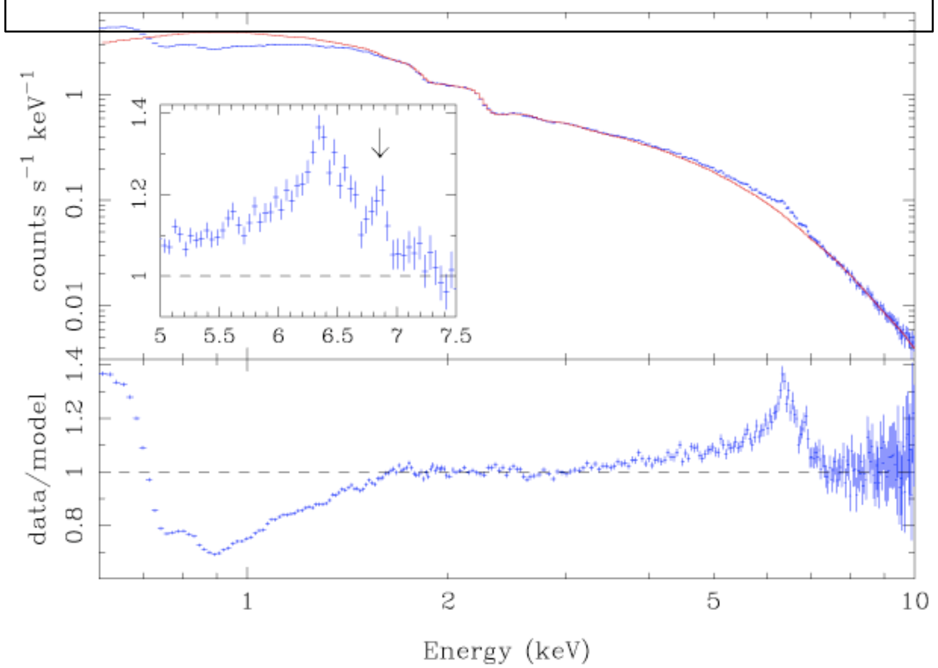


Figure 1. Combined MOS spectrum (the data were combined for plotting purposes only) and ratio of data to a power-law model joining the 2–3 keV data and 7.5–10 keV data. As this is not a realistic model for the continuum the residuals should be considered merely as representative of the spectral complexity. The inset panel shows a close-up of the iron line region with the 6.9-keV feature marked. This figure is available in colour on *Synergy* , in the online version of the journal.

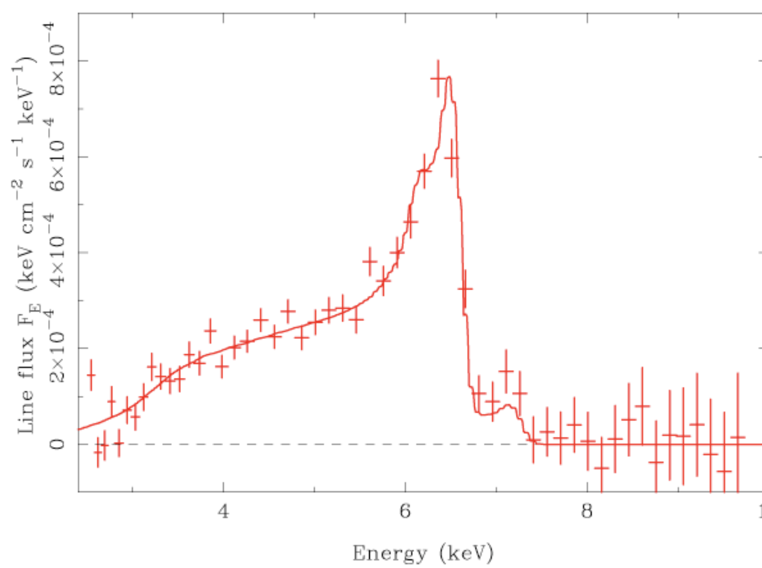


Figure 3. Relativistic iron line profile, shown in (F_ν) flux units, obtained from the ratio of the MOS data to best-fitting underlying continuum model (model 4), multiplied by the continuum model in flux units (as opposed to an 'unfolded' plot). The crosses mark the data points and the solid line marks the line model. This figure is available in colour on *Synergy* , in the online version of the journal.

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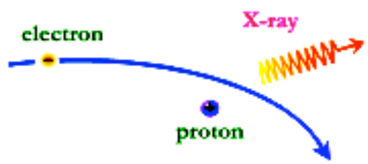

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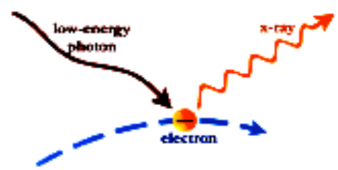

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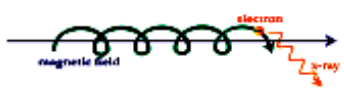

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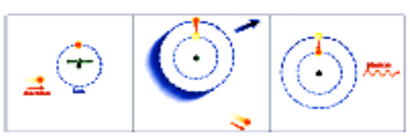
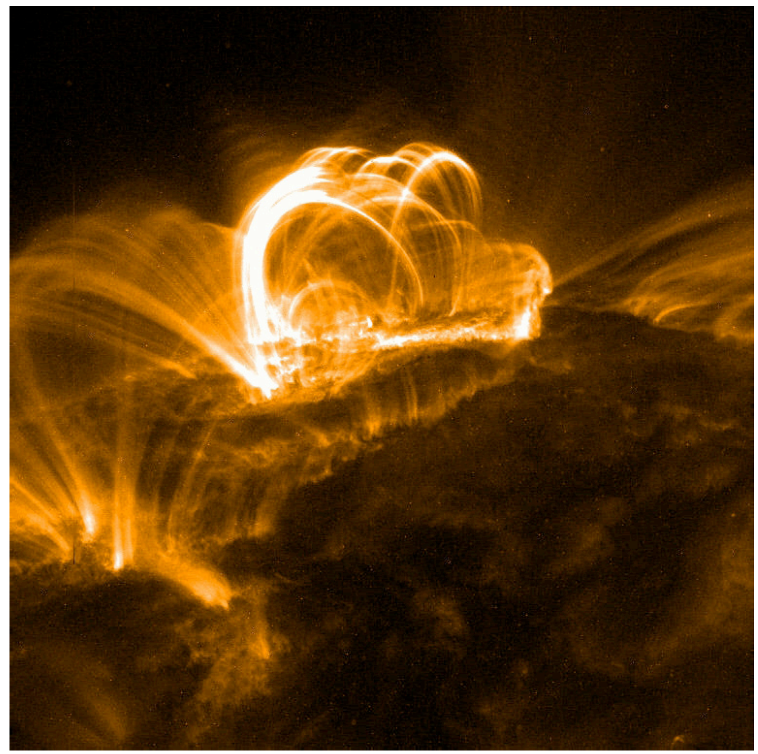


Some X-ray Sources

- Stellar (including solar) coronae



The Sun (with TRACE)

high energy particles → high energy photons

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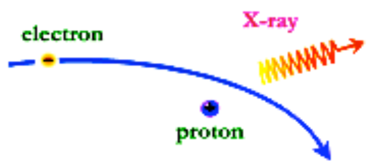

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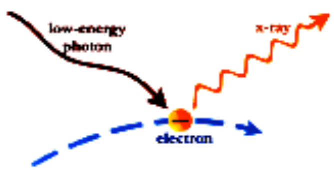

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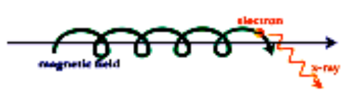

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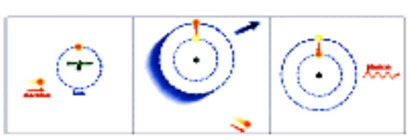

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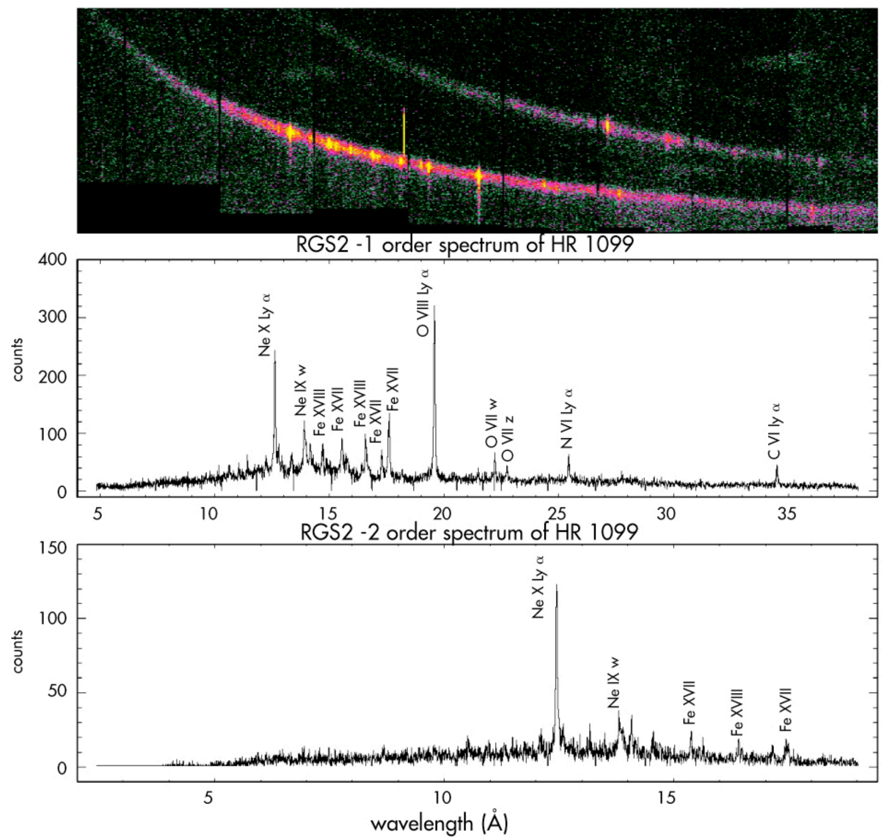

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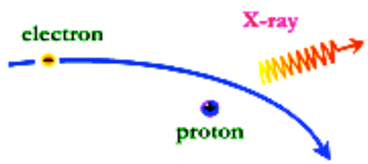

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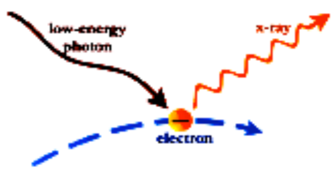

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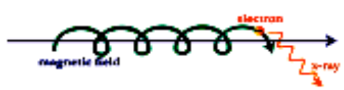

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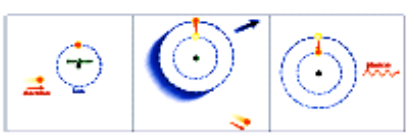
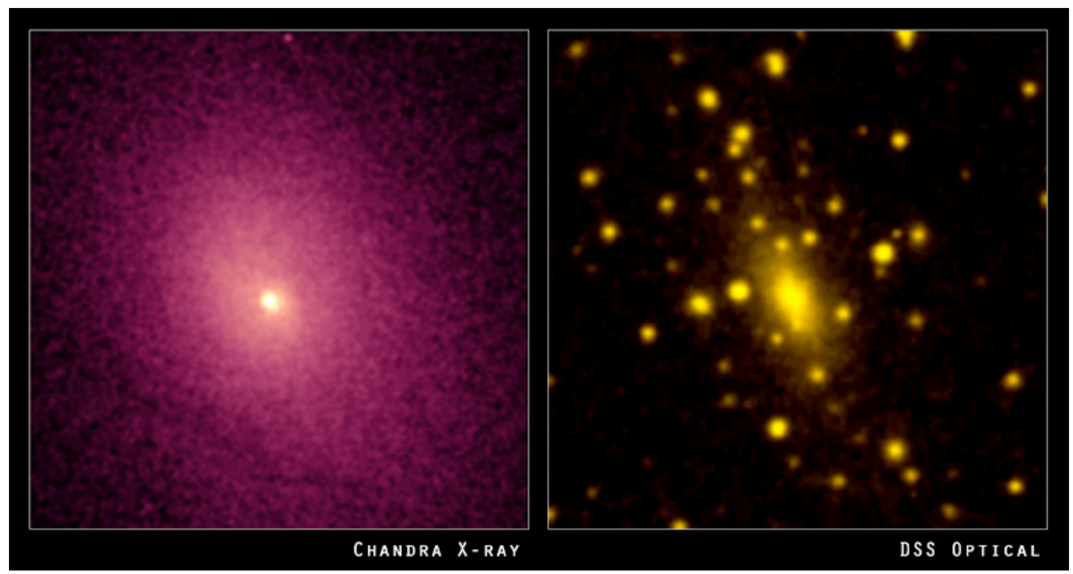


Some X-ray Sources

- Hot thermal plasma in galaxies (including our own) and clusters of galaxies



The Abell 2029 Cluster; X-ray vs Optical

high energy particles ➔ high energy photons

Some *X*-Ray Processes

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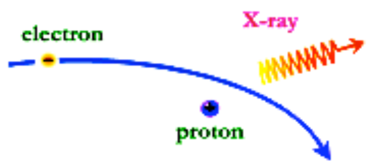

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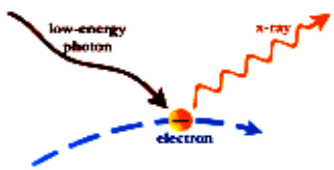

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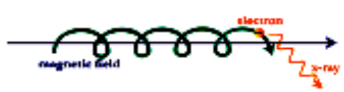

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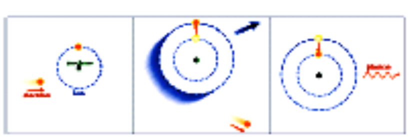

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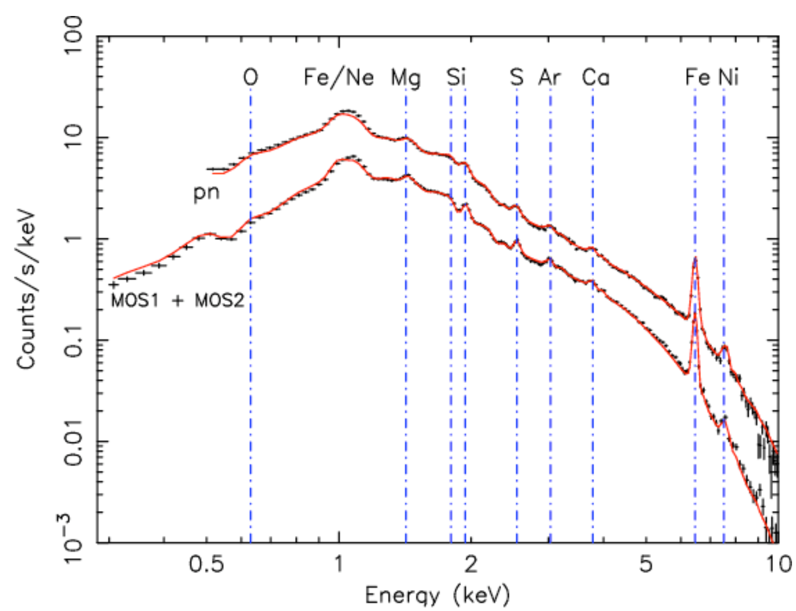
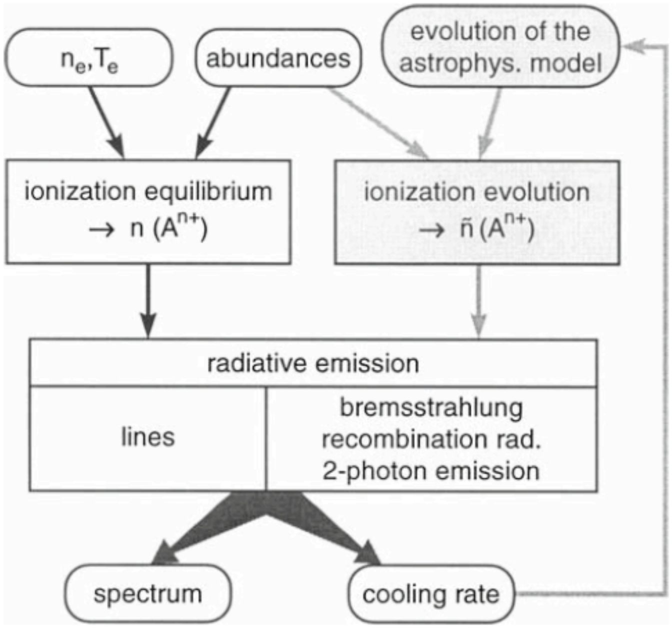
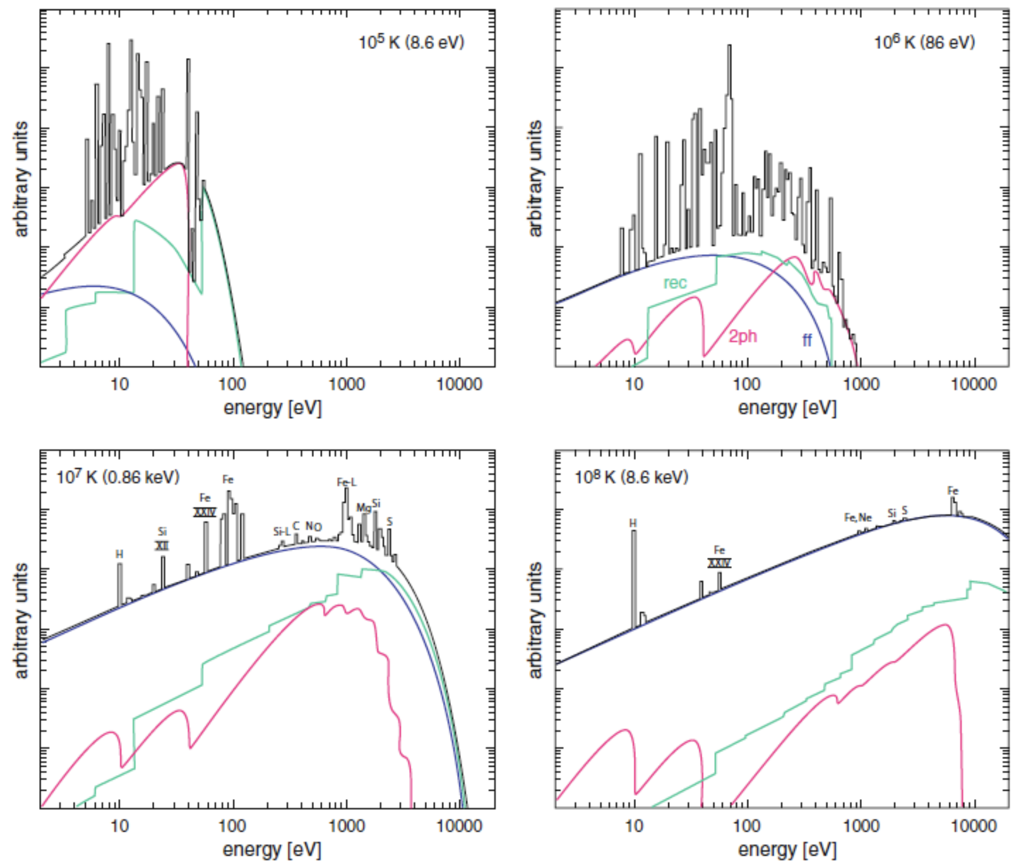
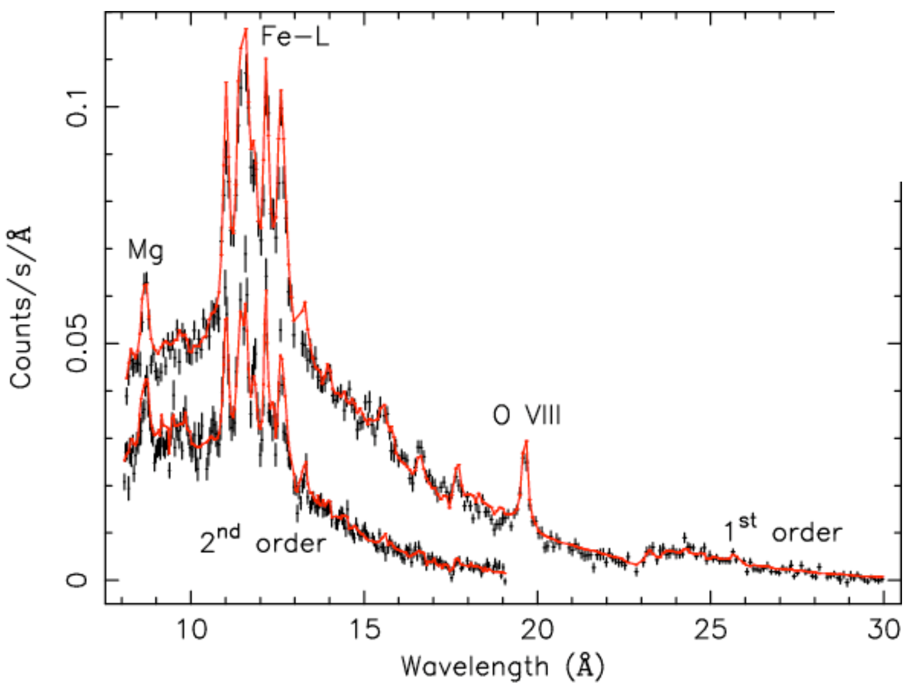
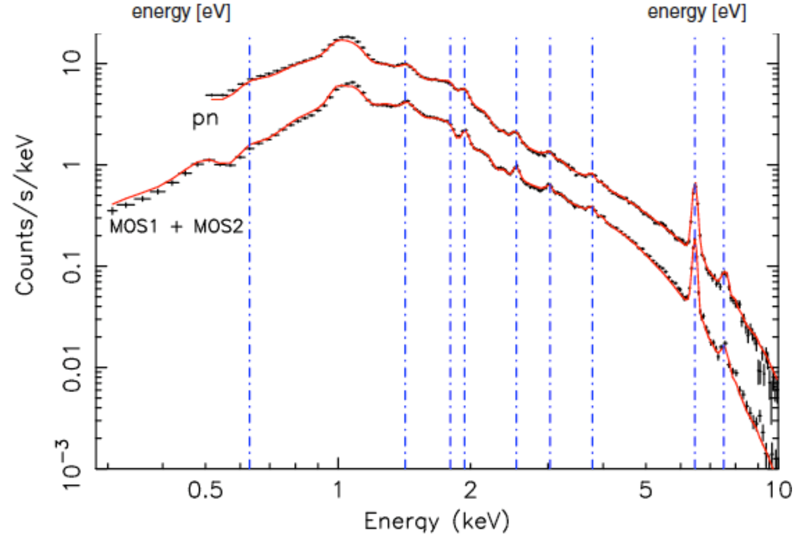


2A 0335+096 galaxy cluster with *XMM-Newton* CCDs

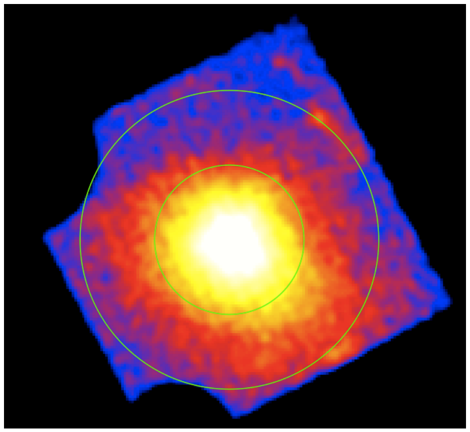

n$_e$,T$_e$
abundances
evolution of the astrophys. model
ionization equilibrium → n (A^{n+})
ionization evolution → ñ (A^{n+})
radiative emission
lines
bremsstrahlung
recombination rad.
2-photon emission
spectrum
cooling rate

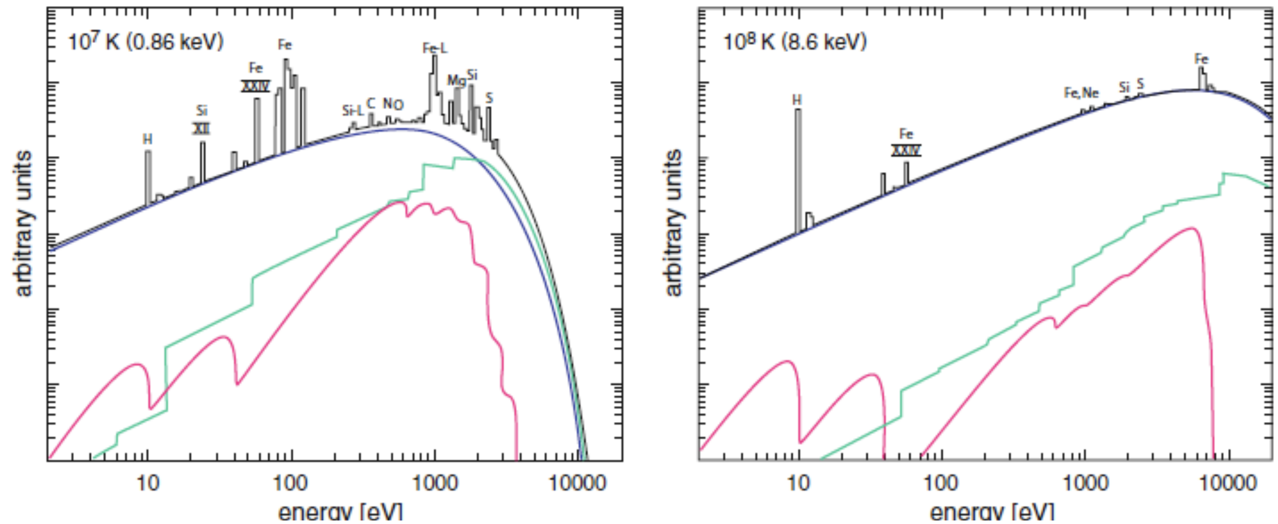

10^5 K (8.6 eV)
10^6 K (86 eV)
10^7 K (0.86 keV)
10^8 K (8.6 keV)
arbitrary units
energy [eV]
10
100
1000
10000
rec
2ph
ff
H
Si
Fe
Fe-L
Mg
S
Fe,Ne

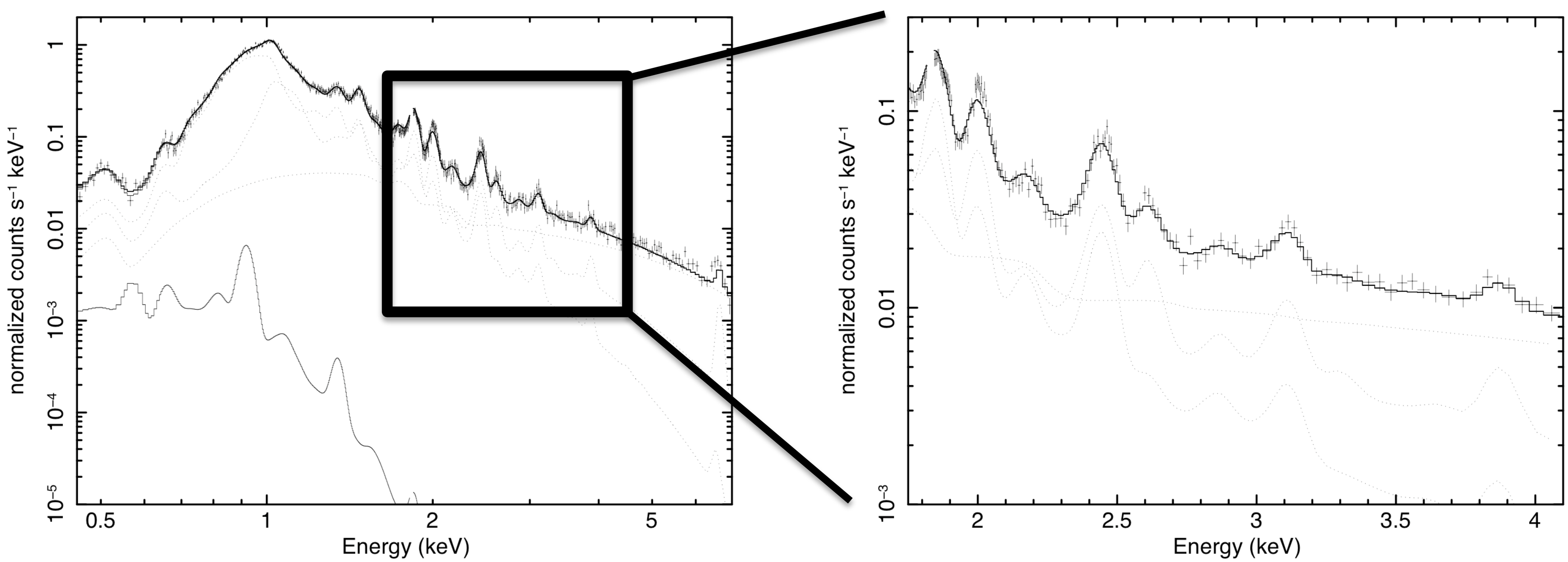

Counts/s/Å
Wavelength (Å)
Mg
Fe−L
O VIII
2nd order
1st order
0
0.05
0.1
10
15
20
25
30


Counts/s/keV
Energy (keV)
pn
MOS1 + MOS2
10^{-3}
0.01
0.1
1
10
0.5
1
2
5
10

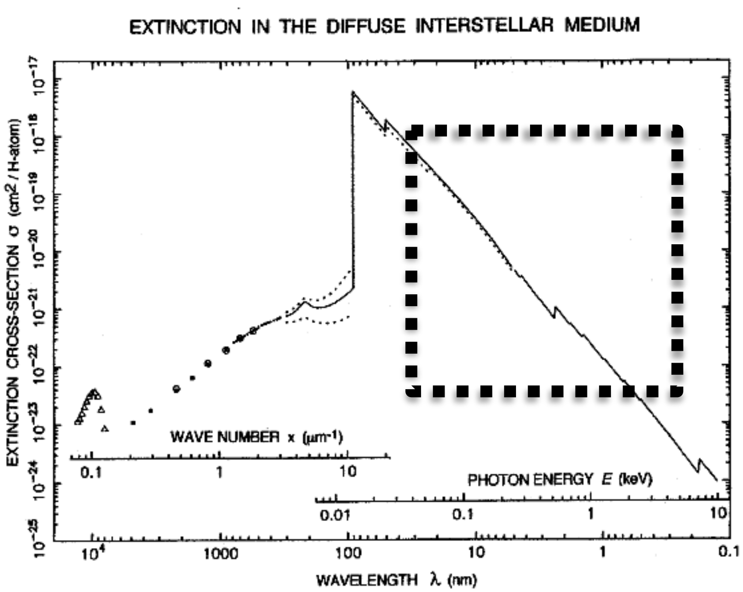
Suzaku XIS1 CCD Spectrum of the NGC 4472 Elliptical Galaxy

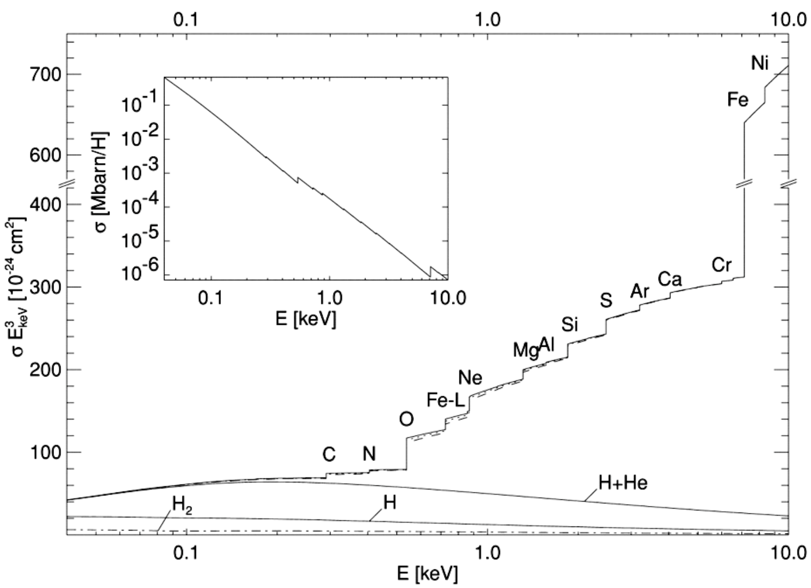






Effect of Absorption

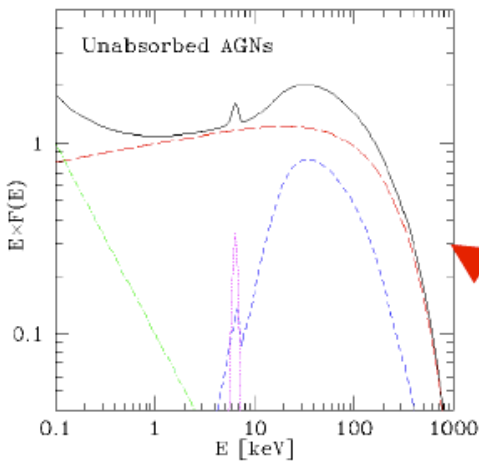


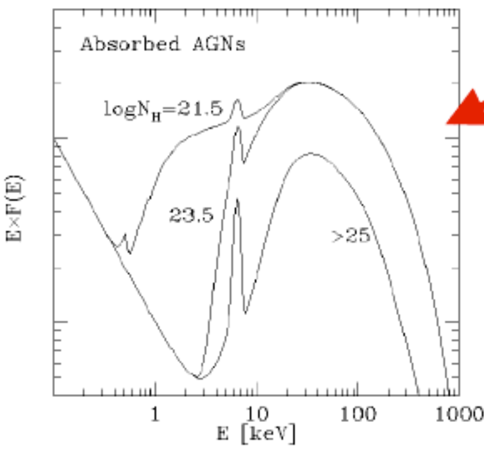


$I_\nu = I_{\nu o} e^{-\tau\nu}$

$\tau_\nu = N_H \sigma_\nu$

$N_H = \int ndl$





The unified model

Antonucci & Miller (1985)

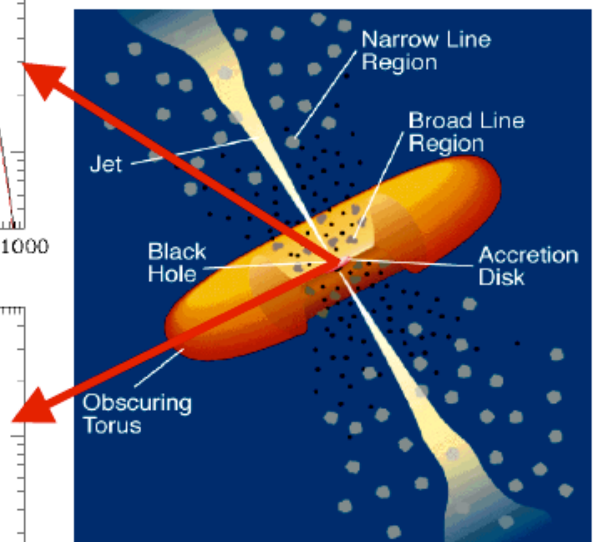
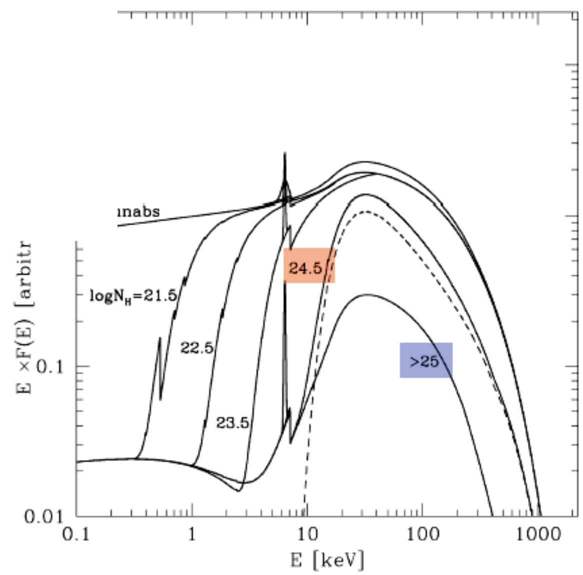


Figure by Urry & Padovani (1995)



X-ray Spectral Analysis Fundamentals

$$C(I) = \int f(E)R(I,E)dE$$

(ignore background for now)

C(I) = counts detected in channel I
f(E) = true flux at energy E (intrinsic spectrum)
R(I,E) = response function
= a(E)r(I,E), a(E) = effective area
r(I,E) =(normalized) redistribution matrix

a(E),r(I,E), and the channel-to-energy conversion are all determined by ***instrument calibration***

X-ray Spectral Fitting

- Hypothesis ➔model of *f(E)* – *M(E)* – *n* physical parameters {*p*} – $M_p(E)$
- Calibrated Response ➔Predicted spectrum $C_p(I)$ for any {*p*}
- Statistical test➔ {*p*} that best describes the data

$$\chi^2 = \sum_{I=1}^{N} (C(I) - C_p(I))^2 / (\sigma(I))^2$$

- *σ(I)=√C(I)* is the standard deviation in the counts in channel *I*
- For the model under consideration, the {*p*} that **minimizes** χ^2 is the **most likely**

X-ray Spectral Fitting

- One may calculate the probability distribution $P(\chi^2/\nu)$ where ν is the number of degrees of freedom, ν=N-n, under the hypothesis that the model is correct. So one can calculate..
  - -- the goodness of fit for any {*p*}
  - -- uncertainties in the form of confidence intervals, since a confidence level corresponds to a given ($\Delta\chi^2$)

Confidence	Parameters		
	1	2	3
0.68	1.00	2.30	3.50
0.90	2.71	4.61	6.25
0.99	6.63	9.21	11.30

Rules of Thumb, etc

- $\chi^2/\nu \approx 1$ for a good fit and "normal errors"

- For all this to work, there must be >>1 count in every bin
  Ignore some bins, group others together

- Adding additional model components can only make the fit better – only justified if it produces a "large" decrease in χ^2
- The "F-test" can be used, under certain conditions, to quantify the whether this is significant.

Spectral Fitting Summary

- The main ingredients of spectral fitting:
  - (a) an observed spectrum (or spectra)
  - (b) the corresponding instrumental responses
  - (c) a set of model spectra
- The steps in model fitting:
  - (a) choose a well-motivated parameterized model (that can characterize the true source spectrum).
  - (b) choose initial values for the model parameters.
  - (c) predict the count spectrum corresponding to these parameters
  - (d) compare the observed and predicted spectra using some statistic
  - (e) search through parameter space until the best match is found

Spectral Fitting Summary, contd.

- Evaluate the model:
  - (a) calculate the "goodness" of the fit in an absolute sense or relative to other models
  - (b) (assuming the model is deemed acceptable) calculate the confidence intervals for the model parameters

The **Xspec** X-Ray spectral fitting package does all this (and more)....

http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/index.html

Xspec Basics:

Getting Help:

- **Quick help**: If you are uncertain about command syntax, typing a command followed by a "?" will print a one-line summary.

- The **help** command :
  XSPEC12> help
  without arguments will bring up the full XSPEC manual in a PDF document, or will open a browser to the XSPEC manual home page either locally or on the HEASARC site.

- Typing
  XSPEC12> help <command>
  will display the manual section corresponding to <command>.

- Help for individual model components can be displayed by
  XSPEC12> help model <modelName>

Commands
XSPEC commands can be divided into 6 categories: Control, Data, Model, Fitting, Plotting and Setting, as follows:

Control commands include items such as controlling logging, obtaining help, executing scripts, and other miscellaneous items to do with the program control rather than manipulating data or theoretical models.

Data commands load spectral data and calibration data such as backgrounds and responses, and specify channel ranges to be fit.

Model commands define and manipulate theoretical models and their parameters, and compute additional information such as fluxes or line identifications.

Fit commands initiate the fitting routines, control the parameter set, perform statistical tests and compute confidence levels.

Plot commands generate about 50 different kinds of 2-dimensional plots

Setting commands change a variety of XSPEC internals which control details of models, statistics, and fitting methods.

A log file of a sample Xspec session, with the commands only -- plus notes.
For more details, see the earlier "Getting Help" slide.

!XSPEC12> show all
Since no files have been read this shows the default setting; generally file and model info is shown.

!XSPEC12> setplot device /xw
Plots appear in an xwindow.

!XSPEC12> setplot energy
Spectra will be plotted versus photon energy (the default is channel #).

!XSPEC12> setplot rebin 5 15
For plotting purposes only, bins are grouped to have a minimum of 5σ significance -- up to a maximum of 15 bins per group.

!XSPEC12> ls
Unix commands such as "ls" may be give directly.

!XSPEC12> data xis1_fak_pi_grp20.fits
Read in the data -- in this case a simulated Suzaku spectrum of an elliptical galaxy, which includes X-ray emission from hot interstellar gas and unresolved X-ray emission.

!XSPEC12> plot efficiency
!XSPEC12> ignore 0.0-0.4
!XSPEC12> ignore 10.0-**
*Ignore energy bins where the effective area ("efficiency") is low; this can also be done in a single line: "ignore 0.0-0.4 10.0-**".*

!XSPEC12> plot ?
What can be plotted?

!XSPEC12> plot data
!XSPEC12> model
What models are available?

!XSPEC12> model wabs*powerlaw
Apply an absorbed power-law model; one may input the default parameters to start with.

!XSPEC12> fit
Press "return" or type "y" when queried to continue fitting; "query y" does this automatically.

!XSPEC12> plot ldata
This is a poor fit, as we knew from the fact that Reduced chi-squared is >>1.

!XSPEC12> model wa*apec
This is a more physically motivated model; apec is a thermal plasma model parameterized by its temperature and metal abundance.

!XSPEC12> fit
The fit is poor.

!XSPEC12> thaw 3
!XSPEC12> fit
By default, the abundance is "frozen" at one; try thawing it and fitting again.

!XSPEC12> plot ldata
Plotting the log of the data shows that the model underestimates the spectrum above 2 keV; this is because we are not accounting for the unresolved X-ray binaries.

!XSPEC12> editmod wa*(pow+apec)
!XSPEC12> freeze 2
!XSPEC12> fit
To account for the binaries add a powerlaw component; the "editmod" command introduces the new model while preserving the parameters of the components that remain; the powerlaw index and norm were given intial values of 1.6 and 0.001 (it is generally a good idea to set the norm of any new component at a relatively small value) and the index is frozen.

!XSPEC12> save model model_1.xcm
!XSPEC12> plot
!XSPEC12> plot ld res
I save this model since the fit was acceptable -- Reduced chi-squared ~ 1 (chi-squared = 1019 for 1052 degrees of freedom).

!XSPEC12> thaw 2
!XSPEC12> fit
!XSPEC12> query yes
!XSPEC12> fit
!XSPEC12> save model model_2.xcm
This is an even better fit (chi-squared = 991 for 1051 degrees of freedom) and I save this model file as well.

!XSPEC12>ftest 991 1051 1019 1052
Since the ftest probability is <<1, this confirms that thawing the powerlaw index resulted in a better fit.

!XSPEC12> editmod wa*(pow+apec+bbody)
Try a more complicated model; for the new blackbody component use 3 keV (the defulat) as the initial temperature and 0.0001 (something small) as the initial norm.

!XSPEC12> freeze 8
!XSPEC12> fit
!XSPEC12> thaw 8
!XSPEC12> fit
!XSPEC12> save model model_3.xcm
!XSPEC12> ftest 988 1049 991 1051

Adding these two new parameters reduced chi-squared by only 3; this is not significant as the ftest indicated.

!XSPEC12> @model_2.xcm
!XSPEC12> save all all_2.xcm

This is the model we adopt; it has thermal plasma ("apec") ISM and non-thermal power-law X-ray Binary components; we save the entire setup in addition to the model.

!XSPEC12> fit
!XSPEC12> error 2
!XSPEC12> save all all_2.xcm
!XSPEC12> save model model_2.xcm

Xspec found a new minimum in estimating the error in the power-law, which we save -- overwriting the old files.

!XSPEC12> err 2.71 2

This gives the 90% confidence range (one parameter of interest) for the power-law index (parameter 2).

!XSPEC12> err 4.61 2 4

This gives the 90% confidence range (two parameters of interest) for the power-law index and plasma temperature.

!XSPEC12> iplot ld res

This starts an interactive plotting of the data (log) and residuals; when the plot looks ok; type "hardcopy" to save is in a postscript file and "quit".

!XSPEC12> mv pgplot.ps simulation.ps

Change the name of the plot.

!XSPEC12> quit