Fundamentals of X-ray Spectroscopy

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> LA-CoNGA (Clase I) Julio 8, 2021

Outline

- Introduction to X-rays
- Fundamentals of X-ray production
- The Fe K line in AGN
- Modeling reflection with/without GR
- Reflexion in Black Hole Binaries
- Reflexion in other sources
- Related Topics

What are X-rays?

High Energy Photons E = 0.1 -- 200 keV Wavelength = 0.1 -- 100 Å T = 10⁶ -- 10¹⁰ K

We can see: Very high temperature Non-thermal particle acceleration Atomic Processes

Discovery of X-rays





Wilhelm Röntgen's first "medical" X-ray, of his wife's hand, taken on 22 December 1895

X-rays in Astronomy



Sco X-I - First X-ray source detected



Number of counts versus azimuth angle (Giacconi et al. 1962)



Temperature and Radiation



Omar, Javier and Margarita at the Aerospace museum.

Planck's Function



Why to Study X-rays?



Why to Study X-rays?



Why to Study X-rays?



Why to Study X-rays?



X-RAY FOCUSING

Requires:

- I. Angle of reflection small related to surface (grazing incidence)
 - ► ~I° for I keV
- 2. Highly **polished surface**
 - ► surface roughness of ~few Å



Slide courtesy of P. Boorman

Supernova remanent Cassiopeia A





Supernova remanent Cassiopeia A





Supernova remanent Cassiopeia A



Optical + X-ray

The Crab Nebula

Infrared





Radio





Visible

X-rays

X-ray Emission Mechanisms

Continuum

Black-Body Bremsstrahlung (free-free) Cyclotron & Synchrotron

Inverse Compton Scattering



Lines

Bound-Bound Fluorescence Charge Exchange Cyclotron Exotic Physics (?)



X-ray Emission Mechanisms

Continuum



X-ray Emission Mechanisms

Lines

Liedahl+Torres05

The X-ray band ($\sim 0.1 - 10$ keV) covers the emission and absorption produced by the inner-shell transitions of the astrophysically abundant ions (C \rightarrow Ni).

- Line positions provide information about the gas composition (identification), as well as about its dynamics (redshifts, gas outflows)
- Line intensities provide information about the column of the absorbing material (including ions), constrains on the ionization degree of the gas ($\xi = L/nR^2$), temperature and density
- Line shapes provide information about the thermal and turbulent motions of the gas, and can also probe relativistic effects near strong gravitational fields

X-ray Emission Lines



Astrophysical Plasmas

In general, there are two types of X-ray emitting plasmas

Collisional:

kT ~ Ionization energy of the ions in the plasma

Photoionized:

kT << lonization energy of the ions in the plasma



Photoionized

T is not a free parameter!

n (or P), abundances

Collisional Plasmas

kT ~ Ionization energy of the ions in the plasma Collisional Radiative:

$Ne = 10^{14} - 10^{27} \text{ cm}^{-3}$

Collisions compete with photons in de-exciting levels. A level with a small A value may be collisionally de-excited before it can radiate

Coronal/Nebular:

Ne < 10¹⁴ - 10¹⁶ cm⁻³

In a Coronal plasma, collisions excite ions but are too rare to de-excite them; decays are purely radiative. This is also called the "ground- state" approximation, as all ions are assumed to be in the ground-state when collisions occur.

Collisional Plasmas

HETG ~500 ks Chandra observation of the accreting young star TW Hydrae (Brickhouse et al 2010)



Spectrum dominated by H- and He-like emission lines

Collisional Plasmas



While the temperature diagnostics for Mg XI, Ne IX, and O VII all give roughly the same result, the density diagnostics are quite different, especially for O VII, leading to the primary result.

Coronal Plasmas

Capella: Active binary system (GI and G8 giants) with a rich spectrum of X-ray emission lines



89 ksec Chandra HETG (Canizares et al. 2000)

X-ray Emission from Capella



MEG, m=-1 : HETGS Spectrum, Capella, Obsid 1103

http://cxc.harvard.edu

Coronal Lines Testing Atomic Data



An unexpectedly low oscillator strength compared to the theoretical calculations has been proposed as the origin of the Fe XVII emission problem (Bernitt et al. 2012)



Photoionized

T is not a free parameter!

n (or P), abundances

Photoionized Plasmas

- Photoionization of plasmas occurs when an external source of radiation illuminates a relatively cold material
- Incident photons excite and/or ionize atoms in the gas
- The gas is heated by photo-absorption or scattering of photons by cold electrons
- Cooling is achieved by both continuum and line emission
- In a photoionized gas, equilibrium is reached at a particular temperature where heating balances cooling

Therefore, the gas temperature needs to be calculated selfconsistently, and the ionization balance is determined by the strength and shape of the incident radiation (for a given density or pressure)

Photoionized Plasmas

- Ionization balance allows for the possibility of different ionic species to co-exist with similar abundances
- Complex emergent spectrum:
 - <u>- Absorption</u>: continuous (photoelectric); discrete (lines, resonances and edges)
 - <u>Emission</u>: continuous (thermal black-body, bremsstrahlung);
 discrete (fluorescence lines, radiative recombination continua)
- Inner-shell ionization and fluorescence emission particularly important for X-ray astrophysics

K-shell Fluorescence



- Needs L-shell electrons
- Photoionization, then either $2p \rightarrow Is$ radiative transition or Auger ionization
- Fluorescence yield ~ Z^4 , appreciable for a high-Z element
- Such a process is an important contributor to iron K emission

Photoionized Plasmas



NGC 3783 900 ksec Chandra observation, over 135 lines identified! Kaspi et al (2003)

Photoionized Gas in NGC 1068



Fits of the XSTAR model to 400 ksec Chandra HETG observation (Kallman et al. 2014)

Photoionized Gas in NGC 1068



- H-like and He-like ions from C to Si, as well as significant emission due to Fe L-shell transitions
- Bright RRC point to the predominance of recombination in a photoionized plasma
- Diversity of ionization parameters ranging from $\xi \sim F_x/n_e = 10$ to 1000.

Plasma Codes

Understanding a plasma requires a physical model. For these, a large number of atomic lines are needed (hundreds or more). Modern plasma codes have made of the hard work, compiling millions of transitions!

Code SPEX Chianti AtomDB

CLOUDY XSTAR

XSPEC ISIS Sherpa Source

http://www.sron.nl/spex http://chiantidatabase.org http://atomdb.org

http://www.nublado.org http://heasarc.nasa.gov/docs/software/xstar/xstar.html

Fitting Codes

https://heasarc.gsfc.nasa.gov/xanadu/xspec/ http://space.mit.edu/asc/isis/ http://cxc.harvard.edu/sherpa/

Summary

Although moderately complex, there are relatively few processes that dominate X-ray emission; analyzing the observed spectrum from each can reveal the underlying parameters. These processes are:

- Line emission
 - Collisional \Rightarrow temperature, abundance, density
 - Photoionized \Rightarrow ionization state, abundance, density
- Synchrotron emission \Rightarrow relativistic electrons, magnetic field
- Inverse Compton scattering \Rightarrow relativistic electrons
- Blackbody \Rightarrow temperature, size of emitting region / distance²
- Absorption \Rightarrow abundance, density, velocity
Einstein and the Space-Time





In 1915 Albert Einstein develops the theory of General Relativity.



The Persistence of Memory, by Salvador Dali

Theoretical prediction of Black Holes



In 1915, provided the first exact solution to the Einstein field equations of general relativity (for non-rotating mass).

"As you see, the war treated me kindly enough, in spite of the heavy gunfire, to allow me to get away from it all and take this walk in the land of your ideas."

- Schwarzschild to Einstein, December 1915.



Accretion Into Compact Objects

1. Material in an accretion disk spirals inward toward the black hole.

Black hole

Fluorescence Lines from the AD disk

2. Most inward motion halts here due to conservation of angular momentum, giving the accretion disk a sharp inner edge.

3. Only part of the infalling material reaches the black hole.

Accretion Physics is the Same!







Neutron Star

Stellar-mass BH

Supermassive BH

Mass of the Compact Object

1.4 - 3 Msun

3 - 100 Msun

10⁶ - 10⁹ Msun

X-ray Reflection First Detections

1960-1970's: First X-ray observatories were launched: *Uhuru, Ariel-V, OSO-8, HEAO-1*.

Several X-ray sources were associated with AGN, with a power-law continuum with Gamma ~ 1.7 (e.g., Tucker et al. 1973; Mushotzky, 1976, 1984).



Ginga Observation of NGC 5548 showing one of the first clear detection of Fe K emission near 6.4 keV (Pounds et al. 1989)



UHURU Observation of NGC 5128 (Tucker et al. 1973)

1980's: Einstein, EXOSTAT, Tenma, Ginga.

Detection of Fe K emission and absorption as a common property of Seyfert galaxies (Pounds et al. 1989, 1990; Matsuola et al. 1990; Nandra & Pounds 1994).

X-ray Reflection First Detections

1990's: ROSAT, ASCA. First CCDs flying on X-ray observatories. First detections of a distorted Fe K line, which was interpreted as emission affected by relativistic effects near the BH (Tanaka et al. 1995; Nandra et al. 1997; Fabian et al. 2000).





Residuals from a power-law fit to the ROSAT spectrum of MCG-6-30-15, showing a strong absorption feature at ~0.8 keV due to iron.

The line profile of iron K-alpha from MCG-6-30-15 observed by the ASCA satellite (Tanaka et al. 1995)

X-ray Reflection from the Inner-Disk

The line profile of iron K-alpha from MCG-6-30-15 observed by the ASCA satellite (Tanaka et al. 1995)

Relativistic Effects (Special + General)



But Why X-ray Reflection is Important?



But Why X-ray Reflection is Important?

X-ray reflection is the corner stone of the Fe-line method to measure the spin of Black Holes





But also see the continuum fitting method in L. Gou's talk tomorrow!



X-ray Reflection from Accretion Disks

The Complex AGN Structure



UNIFICATION





Wavelength



Marin 2016

BROADBAND SPECTRUM



Active Galactic Nucleus



Murphy & Yaqoob (2008)

X-ray Reflection from the Torus

X-rays produced in the central region illuminate the distant torus
The photons excite the cold-neutral material, producing fluorescence (remember the photoelectric effect?)

• Iron K emission is the most prominent (yield $\sim Z^4$)



Suzaku data fitted with the MYTORUS model. The spectral shape depends on the geometry of the system, inclination angle, and column density, providing important diagnostics. See <u>www.mytorus.com</u>

OBSCURATION

COLUMN DENSITY, N_H

Measure of obscuration

C-THICK $N_{\rm H} > 1.5 \times 10^{24} \,{\rm cm}^{-2}$

Slide courtesy of P. Boorman

Video: R. Ramírez

OBSCURED X-RAY SPECTRA



Neutral & Distant Reflection

* PEXRAV (Magdziarz & Zdziarski)
* PEXMON (Nandra)

Provide very simplistic calculation of the reflection spectra. No geometrical information.

* TORUS (Brightman & Nandra)
* MYTORUS (Murphy & Yaqoob)

Provide very simplistic calculation of the reflection spectra, but good geometrical information

- * REFLIONX (Ross & Fabian)
- * XILLVER (Garcia & Kallman)

Provide detailed calculations of the reflection spectra (also including ionization). No geometrical information.

X-ray Reflection from Cold Material

Reflection modeling is being around for a long time...









Current models allow for ionization structure (thus, not so cold material)

Calculation of the Reflected Spectrum

Simplistic assumptions regarding the geometry of the system:

- The illumination is prescribed
- The calculation is done at one single place in the disk
- Gas density is constant in the vertical direction
- No magnetic fields



Ionized Reflection in a Nutshell

In any photo ionized plasma, one needs to solve at least 3 basic equations:

- Level Populations: All processes populating an atomic level are balanced by those depopulating it.
- 2) Energy: All heating processes are balanced with the cooling processes
- 3) <u>Radiation Transport:</u> Interaction of the incident radiation field with the matter in the gas.
- * Incident photons excite and/or ionize atoms in the gas
- * The gas is heated by photo-absorption or scattering of photons by cold electrons
- * Cooling is achieved through both continuum and line emission
- * Equilibrium is reached at a particular temperature where **Heating = Cooling**

* Thus, gas temperature needs to be calculated self-consistently, and the ionization balance is determined by the strength and shape of the radiation field.

The result is a very complex emergent spectrum, with both absorption and emission features!

The XILLVER Code for Ionized Reflection



- Solves the Radiation Transfer equation for every energy and angle at all depths, assuming plane-parallel geometry
- Solves the ionization balance using the XSTAR routines (Kallman & Bautista 2001)
- Includes the most complete and updated atomic data for inner-shell transitions
- Includes Comptonization of the radiation field within the disk

XILLVER: Reflected Spectrum



Input Parameters

<u>lonization</u>: Sets how strong is the illuminating field (Xi = 4pi Fx/ne), where ne=const is the gas density

<u>Gamma</u>: Sets the shape of the incident spectrum by assuming a E[^]-Gamma power-law

<u>Afe</u>: Sets the abundance of iron in Solar units

Gamma=2, log Xi = 2, Afe = 1

XILLVER:Temperature Profiles



XILLVER: Ionization Balance



XILLVER: Ionization Balance

The relative amount of each ion changes with the conditions of the gas



XILLVER: Ionization Balance

The relative amount of each ion changes with the conditions of the gas



XILLVER: Changing the Ionization



XILLVER: Changing the Photon Index

The ionization parameter is the same, yet the changes are dramatic!



XILLVER: Changing the Iron Abundance



The amount of iron (or any other metals) affects both the state of the gas and the spectrum.

Higher Afe increases both the emission and absorption!

XILLVER: The Fe K Emission Complex



The emission of Fe in the 6-8 keV range is due to a large number of transitions

The line energy changes according with the ionization stage



XILLVER: More than Iron









XILLVER: More than Iron





XILLVER: Cold Reflection in IC 4329A



XILLVER: Cold Reflection in IC 4329A


XILLVER: Cold Reflection in IC 4329A



Relativistic effects also need to be accounted for!

Modeling Relativistic Reflection



The relxill model: Combines ionized reflection spectra from xillver (Garcia & Kallman 2010), with the relativistic blurring code relline (Dauser et al. 2010)

> **Reflection fraction** Photon index High energy cutoff Iron abundance

García et al. (2014)



Constraining Physical Quantities



Coronal Height



Inclination



Iron Abundance



Measuring the Spin of Black Holes



Spin Distribution for SMBHs

The distribution of Spin vs Mass can constrain SMBH formation models (Steady Growth/Galaxy Mergers)





Possible observational biases:

- Radiative efficiency scales as ~1/r, which favors high spin detections.
- Also, high spin and low coronae enhances the reflection fraction.

Measuring Spins in BHBs

- BH spins are not always easy to measure. BHBs provide better signal but there are still discrepancies.
- Results often depend on the quality of the data, but also on the quality of the observer ;)



Figure courtesy of J. Tomsick

Compilation from Krawczynski (2018)

The Evolution of the Corona and the Accretion Disk



Coronal Geometry



Non-Static and Extended Corona



Wilkins et al. (2016)





Probe geometry and location of the primary source Low high implies enhanced irradiation of the inner regions



The Reflection Fraction



Photons from the corona can reach the observer, hit the accretion disk, or get lost in the black hole

Dauser, Garcia et al. (2014)

The Reflection Fraction



Dauser, Garcia et al. (2014)

Extreme Reflection in Mrk 335



Extreme Reflection in Mrk 335



Wilkins et al. (2015)

Relativistic Reflection is also important in Stellar-Mass BHs

Black Hole Binaries (BHBs)



- Stellar Masses (~5-30 Msun)
- Modest variability in human timescales
- Many are transient in nature
- They flare in X-rays increasing their luminosity by a billion fold
- An outburst can last from weeks to months
- AU-scale persistent jets and parsec-scale ballistic jets
- X-ray Quasi-Periodic Oscillations (QPOs) (0.01-450 Hz)
- Very distinct spectral states: hard/intermediate/ soft

(Figure courtesy of Jerome Oroz)

RXTE: Rossi X-ray Timing Experiment

Observed hundreds of X-ray sources between December 1995 and January 2012



Proportional Counter Array (PCA)

- Energy range: 2 60 keV
- \bullet Energy resolution: <18% at 6 keV
- Time resolution: 1 microsec
- Detectors: 5 proportional counters
- Collecting area: 6500 square cm
- Layers: 1 Propane veto; 3 Xenon, each split into two; 1 Xenon veto layer
- Sensitivity: 0.1 mCrab

PCA made ~110,000 pointed observations collecting ~295 Msec of data

The Prototypical BHB GX 339-4



Hynes+03: $f(M) = 5.8 \pm 0.5 M_{\odot}$ Kolehmainen+Done10: D = 6 - 15 kpc $M = 6.2 - 15 M_{\odot}$ $20^{\circ} < i < 70^{\circ}$



BHBs in Outburst— GX 339-4



Archival data from the Rossi X-ray Timing Explorer (RXTE)

(Animation courtesy of Navin Sridhar)

BHBs in Outburst— Cyg X-1



The Hard State of GX 339-4



García et al. (2015b)

Disk and Corona Evolution

Relativistic reflection fits of the black hole binary system GX 339-4



Disk and Corona Evolution



For a 10 Solar-mass BH: Delta Rin ~45 km



- Luminosity increases by ~20x
- Rin decreases from a few to ISCO
- Coronal Temp decreases by 10x
- Yet, continuum slope remains the same (r~1.6)... why?

Disk and Corona Evolution

New Black Hole Binary MAXI J1820+70 as seen by NICER



Fits to XTE J1752-223

Similarly to GX 339-4, we find a rapidly spinning black hole $(a^*\sim 0.992)$, also with super-solar iron abundance (Afe~4)



Illumination Geometry

Reflection Spectroscopy of XTE J1752—223:

Highest signal-to-noise reflection spectrum to date (S/N ~ 3000) *** Update: MAXI J1820+70!

Inner-Disk Inclination





García et al. (2018b)

XTE J1550-564 - LOW INCLINATION DISK?



Inclination from reflection modeling inconsistent with radio jet and optical monitoring determinations of the orbital inclination, *i* ~ 40 deg, as opposed to *i* ~ 75 deg (Orosz et al. 2011, Steiner et al. 2012).



Possible misaligned inner accretion region?

Irradiation of Flared Disks



Disk obscuration reduces the blue-wing of the Fe K emission -> Resembles lower inclination! See Taylor & Reynolds (2018)

Obscuration effects:

Under an inclination of **78.5**°, part of the disk is covered, affecting both the line profiles and the time lags



Disk Self Irradiation



Radiation Returning to the Disk due to GR light bending



Flux fraction of returned radiation consistent with ray tracing calculations

Connors, JG,+20

Fe K Reflection in Neutron Stars

Serpens X-1 1.1 1.05 model 1.1 4U 1820-30 Data / Continuum 05 1.1 GX 349+2 1.05 8 Energy (kev)

Iron K lines in three Neutron Stars observed with Suzaku (Cackett et al. 2008) In this case, the Fe K-line provides an estimation of the NS radius, which together with the mass constraints the eq. of state.



Relativistically Blurred Oxygen?

Ultra-Compact X-ray Binaries

Neutron Star

Jet-

Reflected Photon

Compton Scattering of the Infalling Photons

Hot Electrons

C and O-rich No H/He lines

White Dwarf

Disc

Relativistically Blurred Oxygen?

4U 0614+09: Neutron star with a Carbon and Oxygen rich White Dwarf donor.



Chandra spectra shows strong O VIII Ly-alpha emission. Custom-made XILLVER model with low H & He abundances (1% solar) C & O abundances are free parameters

Fits to 4U 0614+091 XMM Data

C & O Abundance: 140 +/- 50 x Solar value Strong Ne K-edge or O VIII K-edge? No neon emission in optical spectra



Madej, Garcia et al. (2014)

Summary

X-ray Reflection Spectroscopy provides one of the most powerful tools to study accreting black holes, with which one can study:

- * The Evolution of Disk and Corona: changes in the corona and accretion disk appear to be correlated. This indicates a connection in the physics that governs the evolution of both structures.
- * **The Spins of Black Holes**: Estimates of **BH spins** for both AGN and BHB are important to understand their formation and evolution history.
- * **The Physics of the accreting flow:** Large iron abundances in reflection measurements are indicative of high-density plasma effects, likely affecting the atomic structure properties.
Escuela Latinoamericana de Relatividad y Astrofísica (ELRA)

Diciembre 1-3, Online

Esta pequeña escuela tiene como objetivo ofrecer cursos introductorios a estudiantes de habla hispana. Los cursos proporcionarán las herramientas más básicas necesarias para iniciarse en la investigación de algunos temas actuales en astrofísica relativista.

La inscripción será gratuita y abierta a toda la región.

Cursos (Sesiones de 45+15)

- * Física de Objetos Compactos (Jorge Rueda (ICRANet))
- * Técnicas estadísticas para el análisis de datos astrofísicos (Cecilia Garraffo (Harvard))
- * Técnicas de análisis espectral en rayos X de objetos compactos (Mariano Mendez (Groningen))

Comité organizador:

Alejandro Cárdenas-Avendaño (Fundación Universitaria Konrad Lorenz/ Princeton University) Javier García (California Institute of Technology) Luis Nuñez (Chair, Universidad Industrial de Santander) Jorge Rueda (International Center for Relativistic Astrophysics)

Adicionales



Some Reflections

- Reflection spectroscopy has proven to be a fantastic tool to study the inner-most regions of accreting sources.
- The state-of-the-art atomic data and modeling tools are allowing us to impose tight constraints on important parameters such as spin, inclination, and Fe abundance.

- The community has played an important role in the improvement of our models:
- I 80 Citing papers
- ~120-140 fits to a single source
- Most of these (~80) are NuSTAR observations!



All of physics is either impossible or trivial. It is impossible until you understand it, and then it becomes trivial. —Ernest Rutherford



Diagnostic Tool: Black Hole Spin



possible **Spin** values: $\mathbf{a} = -1 \dots 1$

a = cJ/GM² (Dimensionless Spin Parameter)

Diagnostic Tool: Emissivity Index



Assumes illumination (and thus emission) follows F~r^e

Diagnostic Tool: Inclination



Inclination mostly affects the blue side of the line

Diagnostic Tool: Emission Angle



Garcia et al. (2014)

RELXILL: The Emission Angle



The reflection spectra differ depending on the Emission Angle

Previous convolution models use Angle Average Spectra

RELXILL: Fits to Ark 120



Suzaku spectrum of the Seyfert I galaxy Ark 120. Solid line is the best fit model with RELXILL.

RELXILL: Fits to Ark 120



The uncertainties are dramatically reduced when the angle-resolved model (solid lines) is implemented.

The Problem of the Iron Abundance

Iron abundance determinations using reflection spectroscopy from publications since 2014 tend to find a few times the Solar value!



High-Density Effects

Models with high gas density ($n_e >> 10^{15}$ cm⁻³) produce a remarkable flux excess at soft energies as free-free emission becomes important.



García et al. (2016a)

High-Density Effects

High-density effects such as continuum lowering could have an impact in the Fe abundance. However, new atomic data for high density plasmas is required!



García et al. (2016a)

The Hardeness-Intensity Diagram



Figure courtesy of Sera Markoff