

**DEVELOPING REALISTIC X-RAY MODELS TO INVESTIGATE THE
CLOSE ENVIRONMENT OF SUPERMASSIVE BLACK HOLES**

TESIS PRESENTADA POR

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A LA

**FACULTAD DE INGENIERÍA Y CIENCIAS
INSTITUTO DE ESTUDIOS ASTROFÍSICOS**

Para optar al Grado de Doctor en Astrofísica

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UNIVERSIDAD DIEGO PORTALES

Santiago, Chile

2025

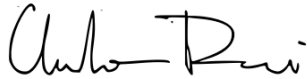
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Acta de Deliberación
Defensa de Tesis Doctoral

En Santiago, el 16 de junio de 2025 el Tribunal de Defensa de Tesis Doctoral compuesto por el Prof. Claudio Ricci (UDP, Chile - Univ. of Geneva, Switzerland), Dra. Chiara Mazzucchelli (UDP, Chile), Dra. Evelyn Johnston (UDP, Chile), Prof. Stéphane Paltani (Univ. of Geneva, Switzerland), Dr. Marko Stalevski (Astronomical Observatory of Belgrade,, Serbia/Univ. of Ghent, Belgium) y Prof. Ioannis Georgantopoulos (National Observatory of Athens, Greece), sobre la base del texto del proyecto, la exposición del doctorando y sus respuestas a las intervenciones de los miembros del tribunal, ha resuelto aprobar la tesis doctoral “Developing realistic X-ray models to investigate the close environment of Supermassive Black Holes” del doctorando Georgios Dimopoulos.

Los miembros del Tribunal firman para constancia.



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To...

my beloved father

Resumen

Esta disertación presenta tres estudios exhaustivos orientados a comprender los entornos más próximos de los agujeros negros supermasivos (SMBH) mediante observaciones y modelización en rayos X. En primer lugar, desarrollamos e implementamos una serie de modelos espectrales de rayos X realistas que tienen en cuenta la compleja geometría y las propiedades físicas del material que rodea a los SMBH. Estos modelos mejoran de forma significativa nuestra capacidad para interpretar los espectros de rayos X de los núcleos activos de galaxias (AGN) y extraer restricciones sólidas sobre las propiedades del medio circunnuclear.

En segundo lugar, investigamos la característica espectral conocida como hombro de Compton en los espectros de rayos X de AGN oscurecidos, lo que aporta información relevante sobre la distribución y las características del material que provoca la ocultación.

Por último, presentamos el proyecto XGATOS, en el que reunimos restricciones observacionales procedentes de datos multiespectrales para construir un modelo espectral de rayos X a medida de la galaxia Seyfert NGC 4941. En conjunto, estos trabajos suponen un avance significativo en nuestra comprensión de la vecindad inmediata de los SMBH, tanto en lo relativo a las condiciones físicas como a la configuración geométrica del medio circunnuclear. Nuestros resultados contribuyen a resolver cuestiones clave sobre la estructura de los AGN.

Abstract

This dissertation presents three comprehensive studies aimed at understanding the close environments of supermassive black holes (SMBHs) through X-ray observations and modeling. First, we develop and implement a series of realistic X-ray spectral models that account for the complex geometry and physical properties of the material surrounding SMBHs. These models significantly improve our ability to interpret X-ray spectra from active galactic nuclei (AGN) and extract meaningful constraints on the properties of the circumnuclear medium. Second, we investigate the Compton shoulder spectral feature in the X-ray spectra of obscured AGN, revealing important insights about the distribution and characteristics of the obscuring material. Finally, we present the XGATOS project, where we collected observational constraints from multiwavelength observations in order to create a tailor-made X-ray spectral model for the Seyfert galaxy NGC 4941. Together, these works constitute a significant advancement in our understanding of the immediate vicinity of SMBHs, in terms of physical conditions and geometrical configuration of the circumnuclear medium. Our findings contribute to resolving key questions about AGN structure.

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Chapter 1

Active Galactic Nuclei: An Overview

The majority of galaxies in the Universe host a supermassive black hole (SMBH) at their centers (e.g., [Kormendy and Richstone 1995](#)), which can have masses $\geq 10^8 M_{\odot}$ (e.g., [McConnell et al. 2011](#); [Woo et al. 2013](#); [Koss et al. 2017](#)). These gigantic black holes can accumulate mass through accretion from the central region of the host galaxy, forming a bright compact source, known as the active galactic nucleus (AGN) ([Haardt and Maraschi 1991](#); [Kuraszkiewicz et al. 2003](#); [Lusso et al. 2012](#); [Koulouridis et al. 2018](#); [Panessa et al. 2022](#)).

Black holes do not emit light by themselves and therefore a more complex mechanism is necessary to produce the radiation observed. As a result, we consider the AGN as the source of the radiation, which consists of a series of structures that contribute to the broadband spectrum. The material closer to the black hole, known as the accretion disk (more details in [Section 1.1.3](#)) contributes significantly in the optical and UV band, whereas more distant dusty media emit in infrared (see, [Section 1.1.5, 1.1.6](#)). The presence of accelerated electrons can lead to synchrotron radiation that enhances the radio emission. The same population of electron can lead to γ -ray emission through the synchrotron-self-Compton mechanism. The nature of AGN expands to multi-messenger phase where neutrinos are expected to originate from such astrophysical objects ([Murase and Stecker 2023](#)).

One ubiquitous characteristic of AGN emission is X-ray radiation. For supermassive black holes, the most common accretion disk model, the SS73 disk (see, [Section 1.1.3](#)), is not capable of producing the X-ray emission we observe in AGN and hence the presence of another mechanism is necessary. The X-ray emission of these AGN is widely accepted to be produced in a

cloud of hot electrons, which upscatters optical and UV photons into the X-ray band through inverse Compton scattering (e.g. [Haardt and Maraschi 1991](#); [Merloni and Fabian 2001](#); [Liu et al. 2015](#)). This population of hot electrons, resides a few gravitational radii above the black hole, and determines the shape of the intrinsic X-ray spectrum (e.g. [Fabian et al. 2009](#)). In [Figure 1.1](#) we show two images of the same galaxy – NGC 3783 – in the optical and X-ray band. On the left, in the optical image, the whole galaxy is visible along with all its features. The stars, as expected, dominate the galaxy in the optical part of the spectrum due to their black body temperature that peaks at the IR, optical, UV and hence, the optical image can be considered ideal for the study of the host galaxy, its shape, and its properties. The morphology of the galaxy, its mass and age can be constrained using optical observations. If we extend our study towards the infrared or UV, properties such as the star-formation of the host galaxy, or the composition of interstellar gas and dust can be derived. Consequently, the light from the central AGN is ”polluted” by the luminous bulge at the center of the galaxy, where a significant amount of stars reside. However, in the image on the right, which is in the X-ray band, the host galaxy disappears since stars and gas clouds do not emit in the X-rays¹ and potential X-ray binaries cannot be as bright as the central AGN. As a result, the nucleus becomes prominent, and therefore the X-ray band is ideal for its study.

AGN emit light in the broadband spectrum that covers the whole spectrum from radio to X-rays and γ -rays. This characteristic introduces criteria that can be used in different bands to categorize AGN. In the optical band, the most widely used categories are Type I and Type II AGN. The main difference between Type I and Type II AGN comes from optical and UV spectroscopy: i) Type I have broad permitted lines (that is, hydrogen recombination lines, intercombination lines, e.g. C IV 1459Å, Mg II 2798Å - and semi-forbidden lines, e.g. C III 1909Å) with line widths of FWHM $\sim 1000 - 10000$ km/s; ii) both Type I and Type II have narrow permitted and forbidden lines: FWHM $\sim 500 - 1000$ km/s. In contrast, Type II AGN lack broad emission lines. These broad emission features imply the presence of gas that revolves around the central black holes at high velocities (e.g., [Wandel et al. 1999](#); [Sulentic et al. 2000](#)). They are produced in the broad line region (BLR), which is expected to be located at distances from the SMBH larger than that of the accretion disk, possibly extending up to the sublimation ra-

¹X-ray emission from hot gas can be found in galaxy clusters.

dus. By examining the velocity-resolved response of the broad lines to continuum variations, the kinematics and geometry of the BLR can be determined (e.g. [Kaspi et al. 2005](#); [Peterson 2006](#)). We present more details of the BLR in Section [1.1.4](#)

In order to successfully describe the spectral properties of AGN, based on the presence or absence of broad emission lines, the AGN Unification Model ([Urry and Padovani 1995](#); [Netzer 2015](#)) was introduced. It suggests that the different types of AGN are fundamentally the same system, and the observed discrepancy is an observational effect that is just the result of the viewing angle. When the AGN is observed pole on, i.e., viewing angles $\sim 0^\circ - 30^\circ$ deg (Type I), there is less material in the line of sight, whereas when observed near edge on (Type II), i.e., $70^\circ - 90^\circ$ deg the dusty torus significantly obscures the inner part of the system (e.g., [Ramos Padilla et al. 2021](#)), which can also be confirmed by the strong absorption that can be detected in the soft X-ray band (e.g., [Awaki et al. 1991](#)). The dusty torus is the key factor of the aforementioned unification model. It is a distribution of molecular gas and dust (e.g. [Wilms et al. 2000](#)) and is expected to be located after the sublimation zone, which can change with the luminosity of the AGN (e.g. [Barvainis 1987, 1992](#); [Ueda et al. 2014](#)) and the Eddington ratio (e.g., [Ricci et al. 2017c](#)). The dusty torus is an important component of AGN

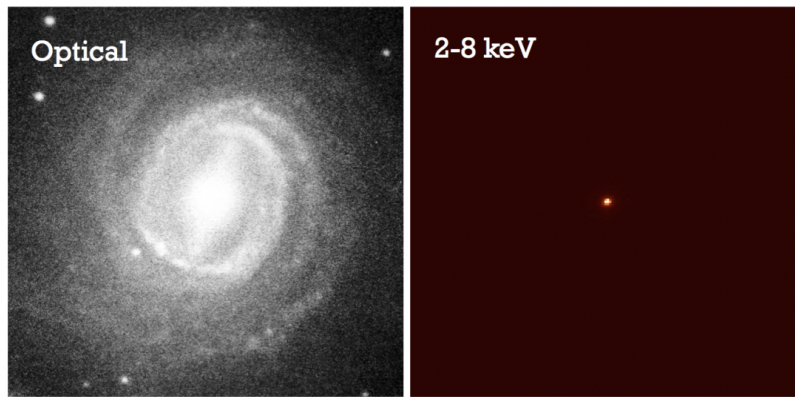


Figure 1.1: Optical and Chandra 2 – 8 keV images of a local active galaxy (NGC 3783); each image is 1.5 arcmin on a side. Note the substantial host-galaxy starlight in the optical band while, in the X-ray band, only the AGN is apparent. The large contrast in the X-ray band between AGN light and starlight helps greatly with the identification of distant AGN. Image from [Brandt and Alexander \(2015\)](#).

and this is illustrated in Section 1.1.5 where we present more details about it. Furthermore, significant efforts have been made to accurately model it as we highlight in Section 1.2.

Different components and different wavelength bands introduce a plethora of criteria that can be used to categorize AGN as seen in Padovani et al. (2017). Therefore, the selection is determined by the physical properties and features to be explored. In Figure 1.3 the SED of a Type I unobscured AGN is shown, where the different components and their origin are illustrated. In the following sections, we will outline the principal elements of an AGN and the physics behind them.

The source of X-rays is located at the core of the system, indicating that X-ray data can examine the near vicinity of SMBH. Although the X-ray emission region is too small to image with current instrumentation, timing analysis and spectroscopy offer ways to probe these regions indirectly. X-ray radiation, along its journey, is subject to interactions from the circum-nuclear material. This interplay between the medium and the photons leaves a footprint on the spectrum in various ways and essentially "breaks" the spectrum into two parts. One part con-

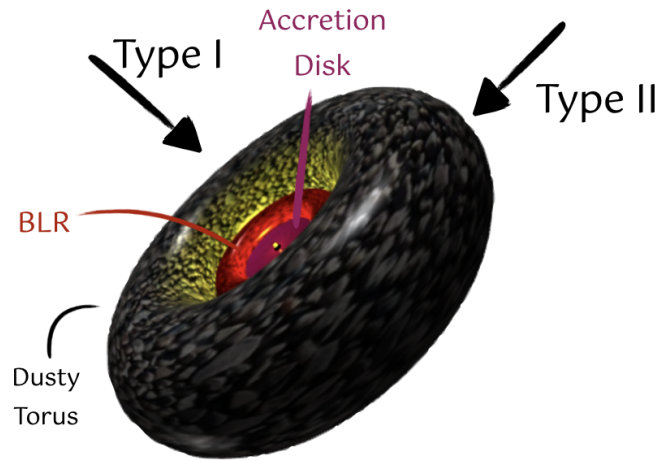


Figure 1.2: A schematic representation of the major components that compose an AGN. The accretion disk provides the necessary photons to the corona so as to generate the X-ray radiation field observed. The gas in the BLR revolves in high velocities and produces broad optical lines and the torus radiates in infrared. The observing angle determines whether the broad lines can be observed (Type I) or not (Type II).

sists of photons that did not interact at all and we refer to it as the *continuum* whereas, the rest of the spectrum compiles the *reprocessed* part of the spectrum usually known as the *reflection* component. The reprocessed part carry signatures of reprocessing in material which can be used to trace its properties from a few hundred gravitational radii to pc scales. The X-ray band will become an even more useful tool for the study of the circumnuclear material of SMBH, with the advent of next-generation X-ray observatories such as *XRISM* ([XRISM Science Team 2020](#)) and *Athena* ([Nandra et al. 2013](#)). The development of new, more realistic, and complex models is crucial to take advantage of these new instruments. In this work, we demonstrate that X-ray spectroscopy, along with realistic geometry models, to shed light on the different components that form an AGN and the physics that drives the phenomena we observe.

In the next chapters, we will dive into the different components that were briefly mentioned and see how they were established as the core of modern AGN models. In Section 1.1.2 the concept of the black hole is introduced, and next we move to the accretion disk in Section 1.1.3. Then, the broad line region is described in Section 1.1.4 and in Section 1.1.5 we present the origin and properties of the dusty torus In Section 1.1.6 is introduced the polar material that recent studies suggest that it is present in most AGN and finally, in Section 1.1.7 is presented the X-ray source and its properties.

1.1 Structure of AGN

1.1.1 The origin of black holes

The origins of a stellar object that is black because of its own gravity are traced back to the 18th century when John Mitchel realized that by using basic Newtonian mechanics on a Sun-like body that is significantly more massive and compact, the escape velocity would exceed the speed of light ([Michell 1784](#)). This idea was later developed by Pierre-Simon Laplace and was called the dark star. In 1915, Albert Einstein published his theory of general relativity, which described gravity as the curvature of spacetime caused by mass and energy ([Einstein 1915](#)). One year later, Karl Schwarzschild found a solution to the Einstein field equations that described the geometry of spacetime around a spherically symmetric mass ([Schwarzschild](#)

1916). The Einstein general relativity along with the solutions of Karl Schwarzschild paved the way for the theoretical exploration of black holes. Later, in the 1930s Subrahmanyan Chandrasekhar showed that a star with a mass greater than the Chandrasekhar limit would form a black hole at the end of its life (Chandrasekhar 1931), a work that led to the physics Nobel prize in 1983 along with William Alfred Fowler. However, for a black hole to be formed, a mechanism was necessary to prove that massive stars can indeed collapse to black holes. A few years after Chandrasekhar, Baade and Zwicky (1934) proposed that compact objects such as neutron stars can be formed as a result of a supernova explosion and the existence of the Chandrasekhar limit ($> 1.4M_{\odot}$) led Sir Arthur Eddington to propose that very massive stars can inevitably collapse to black holes (Eddington 1935). However, the existence of such an exotic object was still under debate until the 1960s and the discovery of quasars by Maarten Schmidt (Schmidt 1963). From the theoretical point of view, the same year Roy Kerr found a solution to the Einstein field equations that described the geometry of spacetime around a rotating mass, a work that led to the rotating uncharged black hole regime, known as Kerr

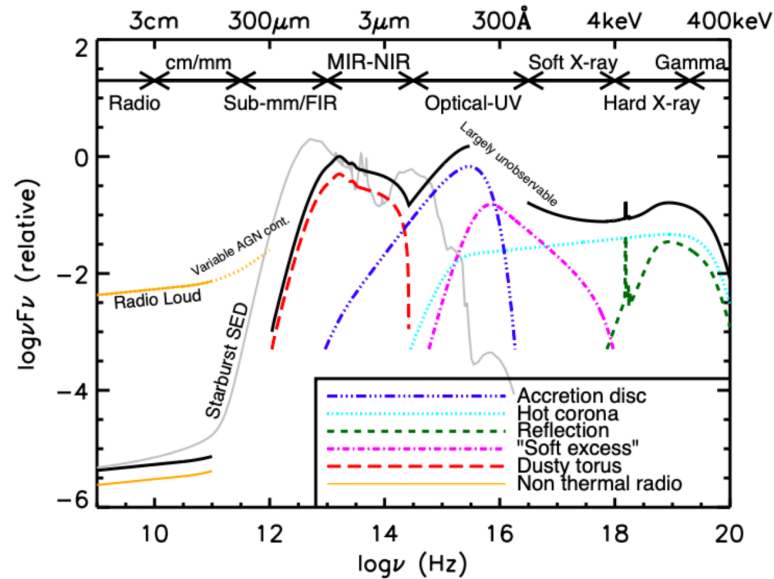


Figure 1.3: A schematic representation of the spectral energy distribution (SED) of an unobscured AGN. The colored curves depict the main physical components of AGN emission, while the SED of a star-forming galaxy is shown in grey. Figure from Harrison (2014).

black holes (Kerr 1963). Newman et al. (1965) extended the solution to charged objects. These two studies established the Kerr-Newman geometry that perfectly describes the gravitational and electromagnetic field around black holes. The first observational hints of the existence of black holes came with the discovery of the Cygnus X-1 binary system, which opened a new field in astronomy (Giacconi et al. 1967; Oda et al. 1971). Ultimately, the discovery of the gravitational waves by the LIGO/Virgo collaboration in 2015, (Abbott et al. 2016) and the direct images from the Event Horizon Telescope (EHT) collaboration of the M87* black hole (Event Horizon Telescope Collaboration et al. 2019), confirmed without any doubt the existence of black holes.

1.1.2 The black holes around us

In summary, black holes are regions of spacetime where gravity is so intense that nothing, not even light, can escape from them. They are the result of gravitational collapse, a process where the gravitational force exceeds any kind of counter-force such as gas pressure or radiation pressure. Gravitational collapse is a fundamental and widespread process in the universe, shaping structures across a vast range of scales. While it is often associated with the formation of black holes – an extreme and relatively rare outcome that typically results from the core-collapse of massive stars in supernova explosions – its role extends far beyond these exceptional events. In the early universe, shortly after the Big Bang, gravitational collapse drove the aggregation of primordial matter into dense clouds, which later gave rise to large-scale structures such as galaxy clusters, individual galaxies, etc. On a more local scale, gravitational collapse is the key mechanism in star formation: vast interstellar gas clouds, under their own self-gravity, contract and fragment to form protostars, ultimately igniting nuclear fusion in stellar cores. When a newborn star, known as Zero Age Main Sequence (ZAMS) star, surpasses a mass of approximately $8M_{\odot}$, its core can eventually exceed the Chandrasekhar limit, and therefore its evolution follows the theoretical predictions for core collapse supernova. At this stage, gravity is sufficiently strong to form a neutron star, which is a spherical entity made up of neutrons. However, for very massive stars ($\sim 20M_{\odot}$), the gravity is so strong that the neutron degeneracy pressure is not enough to counterbalance the gravitational force and the star collapses to a

black hole. This limit is also known as the Tolman-Oppenheimer-Volkoff limit (Tolman 1939; Oppenheimer and Volkoff 1939). These kind of black holes either lurk around us without any evidence or are found in binaries with a companion star, where the accretion of matter from the companion can lead to the formation of an accretion disk and the emission of X-rays, known as X-ray binaries (XRBs).

The category of black holes that is under study in the current work, is known as supermassive black holes. These gargantuan black holes have masses $\geq 10^6 M_\odot$ and their evolution track is still under debate, since they are found across the Universe timescales (e.g., Kovács et al. 2024). Some theories suggest the direct collapse of giant gas clouds, heavy seeding (Bhowmick et al. 2024), while others suggest the growth of stellar black holes through mergers and rapid accretion, light seeding (Ricarte and Natarajan 2018; Mehta et al. 2024).

Finally, there is a third category of black holes, intermediate-mass black holes (IMBHs) with masses $\sim 100 - 1000 M_\odot$. This class of black holes is very elusive and their existence is still under debate, since they are not found at the centers of massive galaxies, nor in X-ray binaries, where the stellar black holes are found. Yet, it is expected to reside in small-scale dwarf galaxies without strong electromagnetic footprint (e.g., Gebhardt et al. 2005; González et al. 2021, see also review Greene et al. 2020).

1.1.3 The accretion disk

The term accretion in astrophysics refers to the process of matter falling onto a massive body. The black holes are perfect examples of massive bodies that have sufficient strong gravitational fields capable of accreting mass from the surrounding media. The infalling material loses gravitational potential energy, which is converted into kinetic energy and radiation. The amount of energy released is related to the attracting object mass and therefore accretion onto compact objects such as black holes, neutron stars, and white dwarfs can be very efficient. In the astrophysical context this effect is responsible for the presence of AGN.

Spherically symmetric accretion, the simplest form of accretion, was initially examined by Bondi (1952) and is known as Bondi accretion. This approach presumes the absence of angular momentum within the system. Consequently, while it serves as a useful approximation, it is

not suitable for situations such as black holes, where accretion disks form.

Accretion disks² are rotating structures of gas and plasma. A particle with angular momentum will orbit the central object in an eccentric path. As long as its angular momentum remains unchanged, the particle will neither fall into the gravitating body nor release its potential energy. In this scenario, no accretion occurs and no energy is emitted. For accretion to occur and for a luminous accretion disk to form, the angular momentum must be transferred outward, allowing the particles to move inward. This process is the result of viscous and frictional forces

²Accretions disks are formed in a variety of astrophysical objects such as protostellar clouds, protoplanetary disks, stars in close binary systems along with the compact objects white dwarves, neutron stars and black holes.

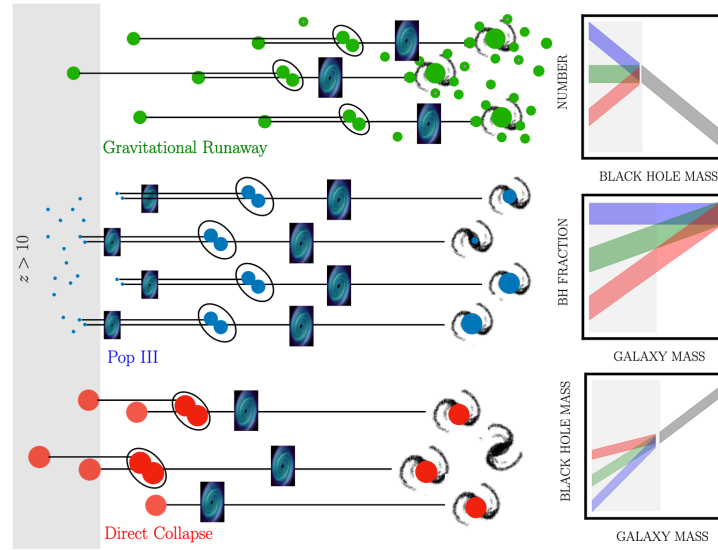


Figure 1.4: Different seeding mechanisms: Seeds formed via early direct collapse (red) or Population III stars (blue) emerge at redshifts $z > 10$, while gravitational runaway processes, e.g. globular clusters, (green) can occur across cosmic history. As cosmic structures evolve, seed black holes undergo mergers (black ovals), generating gravitational waves, and experience accretion episodes (blue disks) that may manifest as active galactic nuclei. By the present day, variations in black hole mass functions, occupation fractions, and black hole-galaxy scaling relations could arise from different seeding mechanisms, illustrated here for nuclear black holes. Grey bars indicate areas where observational constraints remain lacking. Figure from [Greene et al. 2020](#)

that act within the disk, transferring angular momentum outward and allowing the material to fall inward. The energy released in this process is emitted in the form of electromagnetic radiation and can be detected in a wide range of the spectrum (e.g., [Mitsuda et al. 1984](#); [Laor et al. 1997](#); [Done et al. 2012](#); [Vincentelli et al. 2021](#)).

The history of the accretion disk model can be traced back to the 1970s, when Shakura and Sunyaev proposed their disk model ([Shakura and Sunyaev 1973](#)). This milestone work describes the accretion disk onto a compact object and is widely used till today. The model description can be summarized to an optically thick, geometrically thin disk that is in hydrostatic equilibrium and radiates as a blackbody. In their work they assume: 1) the self-gravity of the disk is not important, 2) the disk is axisymmetric, 3) the disk is geometrically thin ($height \ll radius$), 4) the disk is in stationary state ($\partial_t = 0$), 5) the particles follow Keplerian orbits, and 6) the disk is radiatively efficient with the radiation acting as cooling mechanism. Under these assumptions the recipe to describe the accretion disk is simple as long as you follow the conservation of mass, the proper transport of angular momentum, the vertical momentum conservation and the energy balance. The equations describing the disk structure have solutions where the surface density, temperature, and luminosity vary according to a radial power-law. This effectively divides the disk into three distinct regions: the inner region where the radiation pressure is dominant, the outer region where the gas pressure is dominant, and the middle region where the gas pressure and electron scatterings are dominant. The details of the model are found in the original paper as well as in books such as [Kato et al. \(2008\)](#). The work of [Shakura and Sunyaev \(1973\)](#) led to the foundation of the systematic study of accretion disks and is still used today as a reference point for the study of accretion disks, commonly known as the SS73 disk.

The upgrade of the SS73 disk came from [Novikov and Thorne \(1973\)](#) (along with the paper [Page and Thorne 1974](#)) and is known as the Novikov-Thorne disk (NT disk). The main difference between the two models is that the NT disk implements the general relativity effects that are important in the vicinity of a massive object. In their model, they assume a rotating Kerr black hole. They introduced the formalism to describe such systems and they found that the inner edge of the disk is at the innermost stable circular orbit (ISCO) and the disk emits radiation that is redshifted due to the strong gravitational field. Similarly to the SS73 disk, the

NT disk is a geometrically thin, optically thick disk.

Overall, the geometrically thin, optically thick accretion models described above are the most widely used models because they are capable of reproducing the observed properties. However, the temperatures at which the material reaches are not high enough to reproduce the X-rays detected in AGN. [Shapiro et al. \(1976\)](#) explored hot accretion flow for smaller-scale systems and in particular the X-ray binary Cygnus X-1. In contrast to the SMBH, the temperature of the gas is higher and can explain the hard X-ray emission. [Ichimaru \(1977\)](#) extended the work of [Shapiro et al. \(1976\)](#) and introduced the advection dominated accretion flow (ADAF) model. In their description, the energy generated by viscous dissipation can heat the gas instead of being radiated away, a process less efficient yet capable of reaching higher temperatures. ADAF accretion can be found in low-luminosity AGN (LLAGN), X-ray binaries at their hard-low state, etc ([Narayan and Yi 1994](#); [Di Matteo et al. 2000, 1999](#); [Yuan and Narayan 2014](#); [Ruffa et al. 2024](#)).

1.1.4 The broad line region

The accretion disk can extend up to thousands of gravitating radii (e.g. [McHardy et al. 2023](#)), which inevitably raise the question of what follows after it, or the other way around, how the accretion disk is getting fed. The answer to this question is a region that starts from the outskirts of the accretion disk and extends up to what we call the dust sublimation zone, a zone after which dust grains are formed. This region is called the broad line region (BLR). The name coincides with the effect of broad optical line production.

Carl Seyfert ([Seyfert 1943](#)) published a study of six *spiral nebulae*, as they were called back then, reporting the presence of broad optical lines in their spectra. These broad lines were not seen in the spectra of normal galaxies and therefore the presence of them introduced a new class of objects. Even though the terms SMBH and AGN are not mentioned by C. Seyfert, he made the link with the fact that the images of these spiral galaxies host bright nuclei³. Some of the most typical broad lines are the Balmer hydrogen recombination lines H α (6563 Å) and H β (4861 Å), the helium line He II (4686 Å) and the forbidden lines [O III]

³"The widths of the emission bands are probably correlated with the physical properties of the nucleus"

(5007 Å) and [N II] (6584 Å) (Seyfert 1943). High-ionization lines such as Mg II (2798 Å) and CIV (1549 Å) are also present in some AGN spectra (Kriss and Canizares 1982; Wamsteker and Colina 1986). Schmidt (1963) made a breakthrough in understanding quasars⁴ when he identified heavily redshifted Balmer hydrogen lines in the spectrum of quasar 3C 273. This discovery led him to conclude that 3C 273 was not a star, as previously thought, but rather

⁴A terms that refers to active galaxies that appear as point like sources in optical images and therefore can be misinterpreted as stars, quasi-stellar objects.

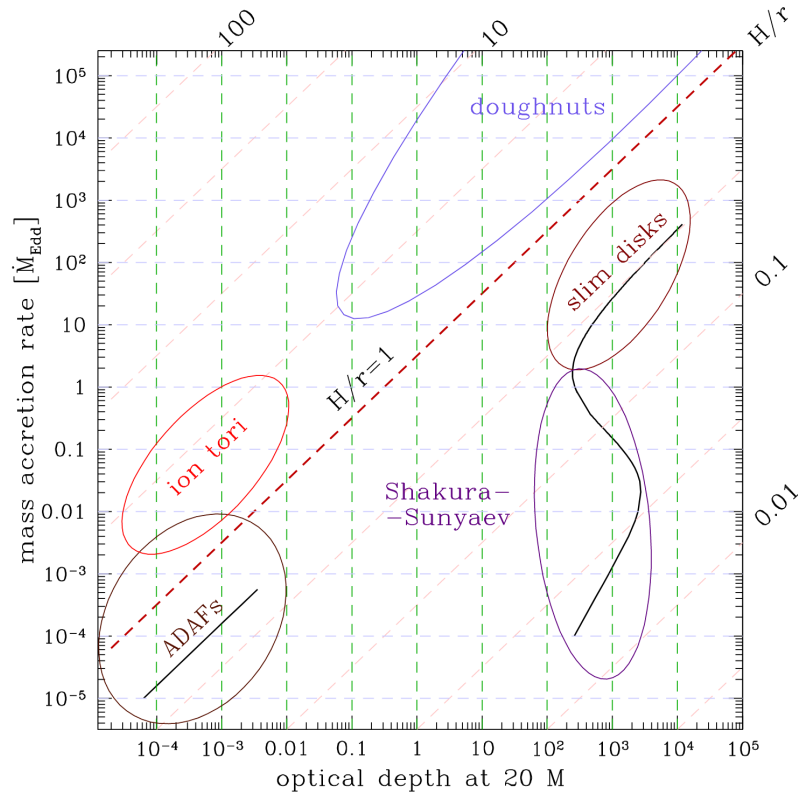


Figure 1.5: An illustration of the different accretion disk models in the parameter space of optical depth and mass accretion rate. The dashed line, $H/r = 1$, depicts the models where the height and radius are equal. Slim disks as expected lie below this line. The figure contains two more models that are not mentioned in this work. The ion tori is a type of accretion introduced by Rees et al. 1982, where a hot torus surrounds the central black hole. The doughnut accretion is a geometrically thick type of accretion described by Abramowicz et al. 1978. Figure from Sadowski 2011

an extremely luminous galactic core located at a great distance. A few years later [Lynden-Bell \(1969\)](#) further developed the idea of the AGN and the quasars, suggesting that the energy source of these objects is the accretion of matter onto a supermassive black hole. The broad lines are the outcome of the material that is in the vicinity of the black hole and is moving at high velocities. [Khachikian and Weedman \(1974\)](#) released their analysis of 71 Seyfert galaxies and for the first time they categorized them into two classes, Seyfert I and Seyfert II, paving the way to the most common classification of AGN until now, based on the presence or absence of broad lines in their spectra. This classification was based on the width of the permitted lines, as type⁵ I galaxies showed Doppler-broadened lines, indicating fast-moving gas near a SMBH, while type II galaxies had narrow lines, suggesting a different physical structure. Osterbrock with two papers studying both Seyfert I and II proposed that the intrinsic difference between the two is the configuration of the material that surrounds the BLR, which sometimes allows them to travel unobscured to the observer whereas sometimes they are absorbed ([Osterbrock 1977, 1981](#)). The concept of one system that has one unique configuration was later supported by [Antonucci and Miller \(1985\)](#) who studied the Seyfert II galaxy NGC 1068 and found that the broad lines are present in the polarized light of the galaxy, suggesting that the broad lines are present but they are obscured by a geometrically and optically thick medium that surrounds the BLR. To sum up, the unification model proposed by [Antonucci \(1993\)](#) and [Urry and Padovani \(1995\)](#), supports that the different types of AGN are fundamentally the same system, and the discrimination is just an observational effect, result of the viewing angle.

The introduction of the BLR concept has been pivotal in AGN research since the 1960s, when broad emission lines were first identified. Over decades, the BLR has remained a key to AGN studies, offering crucial insights into SMBH growth, accretion, and evolution.

The broad lines originating from the BLR are tools of great significance in understanding the properties of the central black hole and the surrounding material. They feature two main characteristics that make them unique. First, the broadening of the lines is linked to the velocity of the gas that emits the line, which is a direct measurement of the gravitational potential of

⁵There is a common interchange in terminology between *type* and *Seyfert*. The *type* term can be used for quasars too that are point like sources, while the term *Seyfert* is used for Seyfert galaxies which are local galaxies that host active nuclei in their centers.

the black hole and hence the black hole mass. To estimate the black hole mass we use the following equation:

$$M_{\text{BH}} = 10^A \left(\frac{L_\lambda}{10^{44} \text{ erg s}^{-1}} \right)^B \left(\frac{\text{FWHM}}{1000 \text{ km s}^{-1}} \right)^C \quad (1.1)$$

where: M_{BH} is the black hole mass in solar masses ($M_\odot$), L_λ is the AGN continuum luminosity at a given wavelength (e.g., 5100Å for H β), FWHM is the full width at half maximum of the broad emission line; A, B, C are empirically calibrated coefficients, depending on the emission line used. This method is widely used in the literature (Koss et al. 2017; Greene and Ho 2005; Trakhtenbrot and Netzer 2012).

The second feature is the time lag between the system's core to the BLR, which serves as

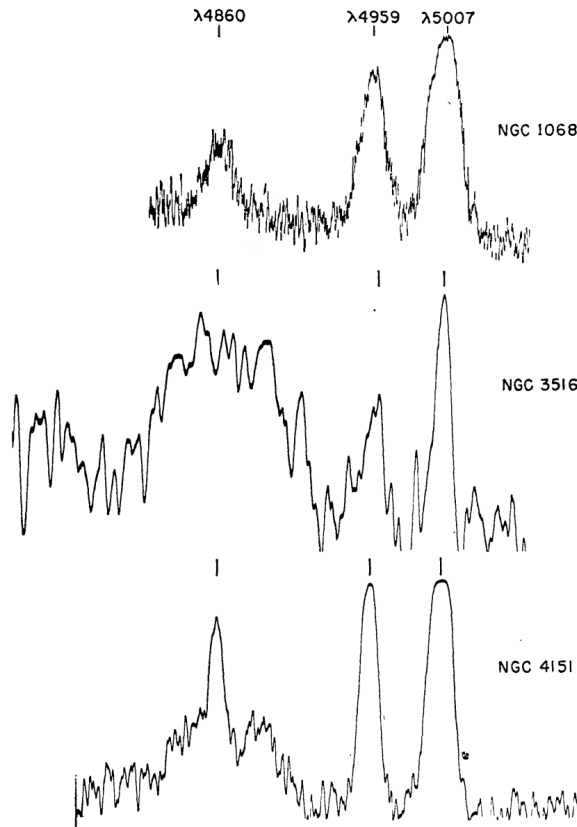


Figure 1.6: The broad lines observed by Clark Seyfert indicating the presence of activity in the nuclei of *spiral nebulae*. The lines are the emission lines $\lambda\lambda$ 4860 (H β), $\lambda\lambda$ 4959 and $\lambda\lambda$ 5007 [O III] in the galaxies NGC 1068, 3516, and 4151. Figure from Seyfert 1943

a tool to determine the BLR's size and consequently, the separation between the BLR and the central black hole (Blandford and McKee 1982; Peterson 1993, 2006). Any variations in the original radiation detected in t_1 , require time $\tau = t_1 + R_{\text{BLR}}/c$ (where R_{BLR} is the distance of the BLR from the central black hole and c the speed of light) to have the equivalent response of the BLR. Considering that the material is virialized, this variation can be directly linked to the black hole mass via:

$$M_{\text{BH}} = f \frac{R_{\text{BLR}} v^2}{G} \quad (1.2)$$

This technique is known as reverberation mapping. The distance from where most of the BLR flux originates is linked with the luminosity of the central engine. Various works propose the *luminosity - distance* relation (Bentz et al. 2013; Kaspi et al. 2000, 2005), such as:

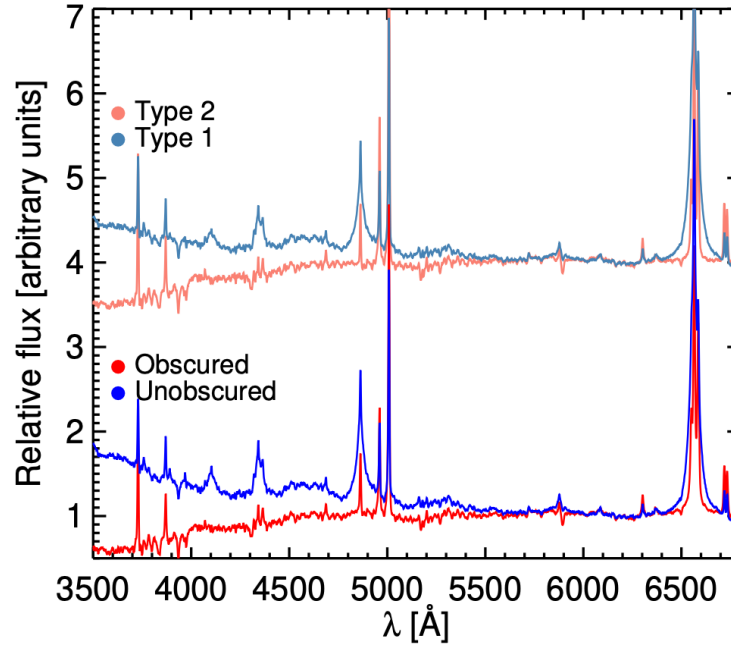


Figure 1.7: An example of type I and type II spectra of AGN. The type I spectrum is characterized by the presence of broad lines, while the type II spectrum shows only narrow lines. The spectra are median composite rest-frame spectra of WISE-selected obscured and unobscured AGN compared to spectroscopic Type 1 and 2 sources. Figure from DiPompeo et al. 2018

$$\frac{R_{\text{BLR}}}{10 \text{ lt-days}} = (2.23 \pm 0.21) \left[\frac{\lambda L_{\lambda}(5100 \text{ \AA})}{10^{44} \text{ ergs s}^{-1}} \right]^{0.69 \pm 0.05} \quad (1.3)$$

For nearby sources, more sophisticated techniques with advanced interferometry instruments provide direct measurements of the boundaries of the BLR. The GRAVITY instrument on the Very Large Telescope Interferometer (VLTI) was used to measure the size of 3C 273 (Gravity Collaboration et al. 2018). Several sources have been later studied with the same instruments that provide statistical results for the size of the BLR (e.g., GRAVITY Collaboration et al. 2020a, 2021).

1.1.5 The torus

The discovery of broad lines was a pivotal moment for the study of AGN. The categorization into type I and type II that was described in the previous paragraph helped to a more systematic approach. However, the cornerstone of that theory was the unification model, and even though it was clear that the presence or absence of broad lines is the key factor for the two categories, there was one thing that was left to be settled. The obscurer of the broad lines. A toroidal structure is widely accepted as the main obscurer of the central source (e.g., Antonucci and Miller 1985; Antonucci 1993; Urry and Padovani 1995). It is found after the sublimation zone and consists of a mixture of gas and dust, which contributes significantly to the submillimeter and infrared bands due to its temperature. In the same period, theoretical advancements were made in order to explore whether a toroidal structure that surrounds the central region can in fact be stable. Krolik and Begelman (1988) explored the energetic and dynamic part that is responsible for the formation of a structure composed of molecular clouds. Later, using this theoretical model, they tried to reproduce infrared spectra that are expected to be emitted by such a torus (Pier and Krolik 1992). They presented in detail the emergent spectrum for different dust temperatures and observing angles. Lawrence (1987) explored all the phenomenological features of AGN at that time and tried to do a comprehensive classification of the different types of AGN. A few years later, a dedicated work focused on the tori of AGN was published that suggested that the material that forms the torus does not necessarily originate from the host galaxy and move inward, but it can be a result of winds that expel material

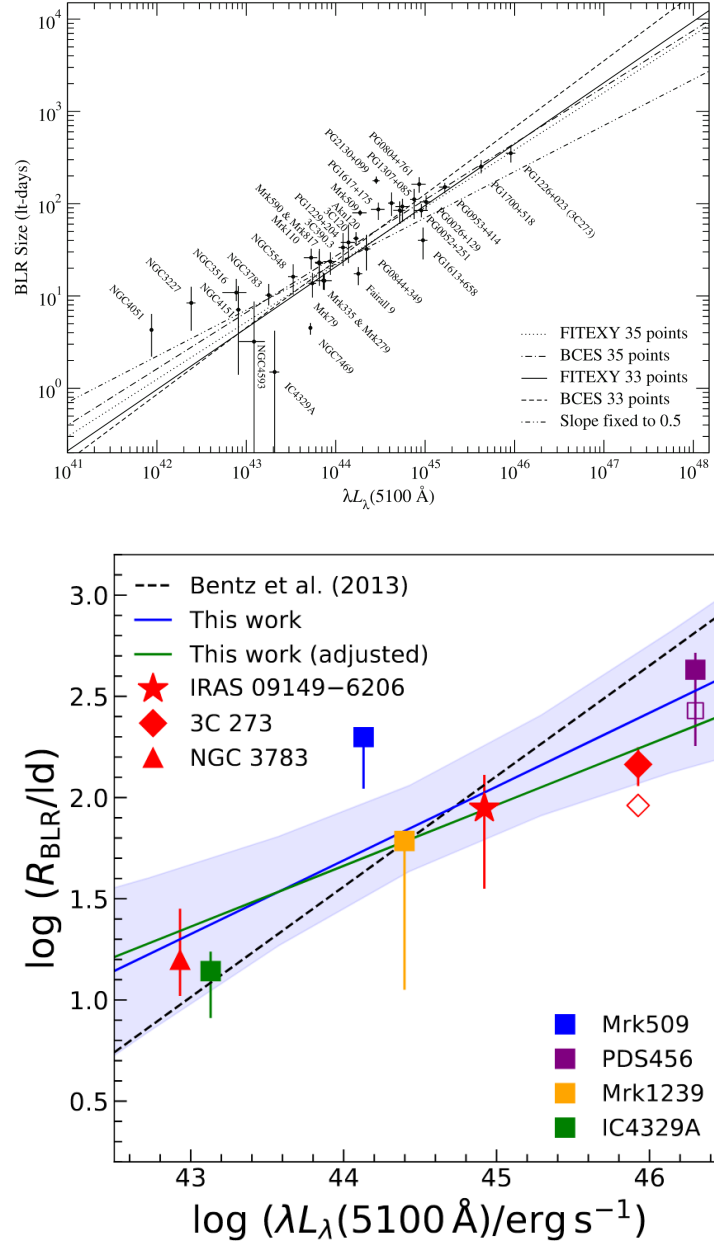


Figure 1.8: *Top:* The size of the BLR in light days Balmer line averaged vs the $\lambda L_{\lambda}(5100 \text{ \AA})$ luminosity (erg/s). The BLR size of each data set is determined from the averaged Balmer line time lags. Figure from [Kaspi et al. 2005](#). *Bottom:* Similar scaling relation figure, this time based on the interferometric data provided by GRAVITY. Figure from [GRAVITY Collaboration et al. \(2024a\)](#)

from the inner parts outward, which then cools down and settles there (e.g., [Lawrence 1991](#); [Wada 2012](#)). This gave a more dynamical view of the torus and its formation, which has been supported by contemporary studies as well (e.g., [Venantzi et al. 2020](#)). Although the dominant theory back then suggested that the torus is a smooth and homogeneous structure, the IR radiative transfer work of [Granato and Danese \(1994\)](#) that covered the SED of Seyfert 1 and 2 AGN from 0.1 to 1000 μm , suggested that the torus needs to have different zones where different dust particles are formed or evaporated, to reproduce the silicate features observed. More recently, in one of the first interferometric studies of the torus, [Tristram et al. \(2007\)](#) used the VLTI MIDI instrument to study the Circinus galaxy and found that in order to reproduce the observed visibilities⁶ the torus must be clumpy. The clumpy torus model has been widely used in the literature since then and is considered one of the most realistic torus models (e.g., [Nenkova et al. 2008a,b](#); [Ramos Almeida et al. 2009](#)). Facilities such as GRAVITY and MATISSE yield data with exceptional resolution for nearby objects like NGC 1068, aiding in the mapping of the dusty medium. These findings question the unified model by indicating more complex arrangements. They reveal a compact equatorial disk along with an extended polar component, which implies a more intricate geometry than was once believed (e.g., [Leftley et al. 2024](#)). In the next section we will illustrate in more detail the dusty polar medium.

In the X-ray domain, the torus is responsible for the absorption of the X-ray radiation that is emitted. [Mushotzky et al. \(1993\)](#) highlighted the importance of the cold torus around the SMBH, which in different types of AGN contributes with various features such as emission lines, absorption of soft X-rays, the Compton hump, etc. In Figure 1.9 is presented the model of [Mushotzky et al. \(1993\)](#) that shows the different AGN components and the role of the torus in the X-rays.

Using archival data [Risaliti et al. \(2002\)](#) studied the variability of 25 Seyfert II galaxies, showing that changes in the line-of-sight column density can be attributed to the structure of the torus, which is expected to have clouds of various densities that obscure the X-ray source at certain periods. More recent work suggests that variability can be linked to material that can be found in different radii from the center and can be attributed to various components (e.g.,

⁶In optical/infrared interferometry, visibilities describe how "resolved" a source is when observed with a specific baseline (i.e., a telescope pair). They are essentially a measure of fringe contrast.

Bianchi et al. 2012; Rivers et al. 2015). With the advent of the X-ray observatories Chandra and XMM-Newton the study of the torus, via the X-ray spectrum and the reflection features that it produces, advanced significantly (e.g., Young et al. 2001; Molendi et al. 2003; Matt et al. 2004; Akylas and Georgantopoulos 2009).

In summary, a combination of observations and theoretical work has led to the understanding that the torus is a key AGN component, responsible for the obscuration. The torus is a complex structure that is not necessarily smooth and homogeneous but rather clumpy and dynamic. The torus is responsible for the absorption of the X-ray radiation as well as its reflection.

1.1.6 The polar material

Recent high-resolution infrared (IR) observations have uncovered an additional component, the polar dusty medium, which often is described with a conical shape (e.g., Stalevski et al. 2017; Leftley et al. 2024). This discovery challenges the archetype of the unified model. The compact scale of the medium near the SMBH made it challenging for astronomers to study the polar material. Extended emission has been found in a handful of AGN, with the most prominent example being the Circinus galaxy and NGC 1068. Raban et al. (2009) studied

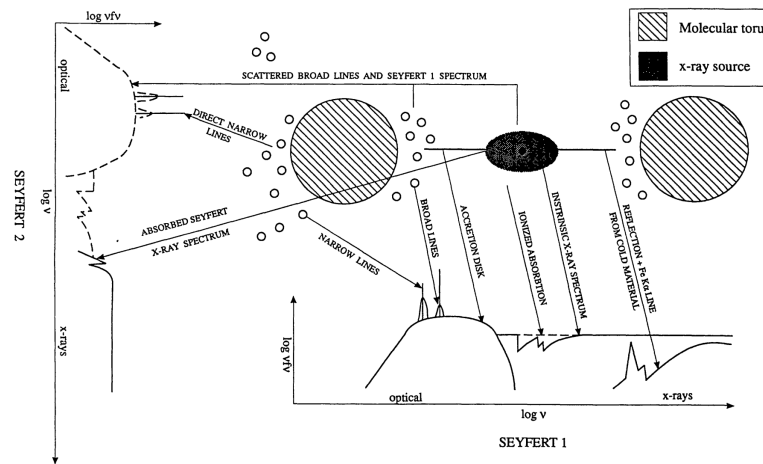


Figure 1.9: The model of the AGN that is presented in Mushotzky et al. (1993). The torus is the structure that surrounds the central black hole and it is responsible for the absorption and reflection of the X-ray radiation that is emitted by the source. Figure from Mushotzky et al. 1993.

NGC 1068 using the MIDI instrument and reported that although the dusty torus is resolved, known as *component 1*, there is strong evidence of a second component, also dusty, that is located at the polar region of the source, *component 2*. This paved the way for the first hints of the presence of the polar dusty material in the AGN. These findings were identified as a defining attribute of NGC 1068 in a study by [López-Gonzaga et al. \(2014\)](#), which used the same instrument to demonstrate that the polar dusty material is not only present, but also contributes four times more to the mid-infrared flux at $12\mu\text{m}$ than the central dust. Similarly to NGC 1068, the Circinus galaxy has been studied in detail in the IR and the presence of polar dust has been confirmed ([Tristram et al. 2007, 2014](#)). Using the VLT/VISIR instruments and high-fidelity N-band images of the Circinus galaxy, [Stalevski et al. \(2017\)](#) identified a polar dusty hollow cone that extends up to 40 pc perpendicular to the SMBH, accretion disk, and torus. The authors managed to disentangle the contribution of the torus and the polar material, suggesting that there is a tilted disk that illuminates the polar structure and consists of a conical shell (hollow cone) of given opening angle and angular width. This conical or hyperboloid shell reproduces not only the observed images but also the observed SED of the source.

[Asmus \(2019\)](#) released the study of 9 [O IV] bright AGN, observed with the VLT/VISIR instrument. All of these sources show strong polar emission. The author found evidence of such emission in all but one source (see Figure 1.10), revealing that the polar dust has to be optically thin on average, which explains, the small dispersion in the observed mid-infrared vs X-ray luminosity correlation. This work suggests that the polar dusty medium is not a rare phenomenon that is present in a few sources, but rather a common structure that is present in most AGN.

[García-Burillo et al. \(2021\)](#) studied comprehensively the extended material around AGN using ALMA in both the dust continuum (351 GHz) as well as the molecular CO(3-2) line. The authors found that the extended material is present in all sources further supporting the presence of polar dusty media in AGN. In a follow-up paper, [Alonso-Herrero et al. \(2021\)](#), using IR observations they tried to map this polar emission and disentangle it with the torus emission. Furthermore, the analyzed sources were placed in the parameter space of the Eddington ratio and column density, divided into distinct regions. Some of these regions were occupied by AGN featuring polar extended emission, pointing towards a relation between the presence of

polar material and these AGN properties. In a theoretical work, [Venanzi et al. \(2020\)](#) suggested a blowout region that is responsible for the formation of the polar material (see Figure 1.11). The interplay between the covering factor of the obscuring material and the SMBH accretion rate has been proposed as a key factor that highlights the dynamic evolution of AGN ([Ricci et al. 2017d](#); [Ramos Almeida and Ricci 2017](#)).

1.1.7 The X-ray source

AGN are well-known for the emission of light across the electromagnetic spectrum, from radio to gamma-rays as illustrated nicely in Figure 1.3. However, they gain popularity due to their notable X-ray emission, which stands out when identifying them (see, Figure 1.1).

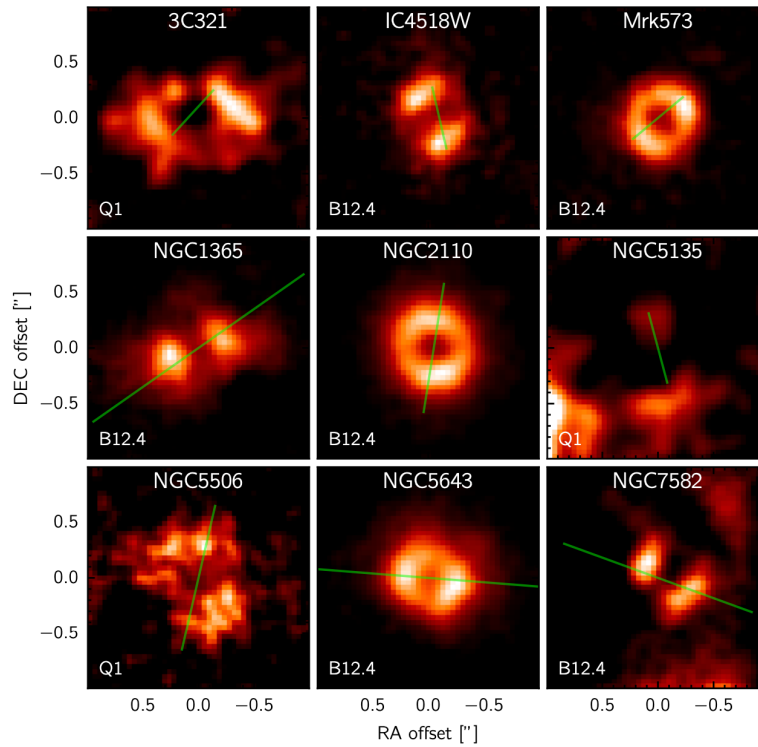


Figure 1.10: The polar dusty medium that is present in the AGN. VISIR images zoomed in $2'' \times 2''$ with the central point source subtracted with the corresponding PSF. The green line in each image marks the system axis PA and has a length of 200 pc at the source distant (except for 3C 321 where it is 1 kpc). For details see the original paper. Figure from [Asmus \(2019\)](#)

Even though extraterrestrial sources dominate the X-ray universe, the origin of X-rays begins in the 19th century with the discovery of X-rays by Wilhelm Röntgen in 1895, which resulted in the very first Nobel prize in 1901. Due to the fact that the Earth's atmosphere absorbs X-rays, it was not until the 1960s that the first X-ray sources were discovered. In 1962, a team led by Riccardo Giacconi (Nobel 2002) made a discovery when their detectors revealed a bright X-ray source known as Scorpius X-1 (Giacconi et al. 1962). This source, far exceeding the X-ray output of the Sun, was the first convincing evidence that the high-energy universe contained a powerful extrasolar source, opening the door for X-ray astronomy (Giacconi et al. 1967). In the years following, Giacconi's role in establishing X-ray astronomy was a key factor. Recognizing the need for more observations, he contributed to the development and launch of dedicated X-ray satellites such as Uhuru (launched in 1970), which conducted an all-sky survey and cataloged hundreds of X-ray sources (Giacconi et al. 1971). His contributions extended to later missions like the Einstein Observatory and paved the way for modern observatories (e.g., Chandra and XMM-Newton), all of which have provided deeper insights into the physics of

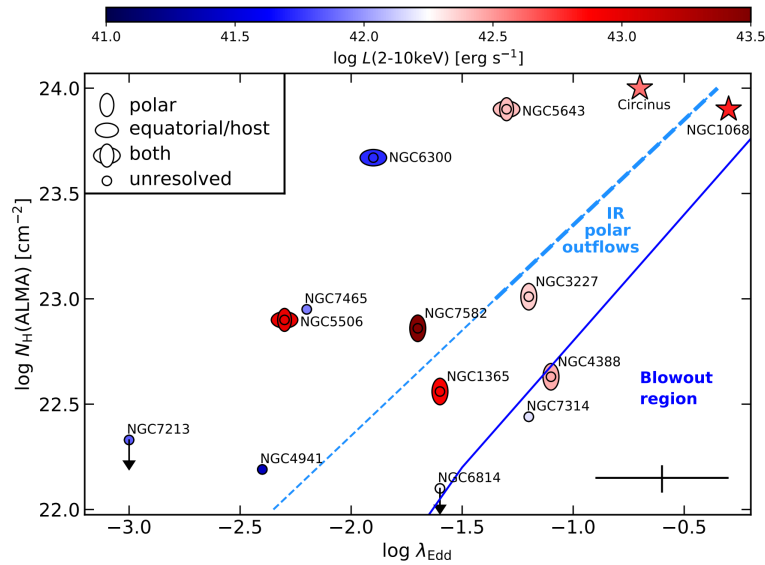


Figure 1.11: The parameter space of the sources studied by Alonso-Herrero et al. (2021). The sources are divided into regions based on the Eddington ratio and the column density. The sources that host polar extended emission are marked with the red circles. Figure from Alonso-Herrero et al. 2021

extreme environments such as those surrounding black holes.

This new exciting domain of astrophysics that emerged from the discovery of X-rays from outer space gave boost to the theoretical work that aimed to explain the physical processes that are responsible for the X-ray emission. From the early 60s to the late 90s a series of works have been published that slowly evolved to incorporate more complex physical processes in order to understand the variety of observations available. Observations got better and better as newer observatories were launched. A cornerstone of how light interacts in astrophysical sources is the book by [Rybicki and Lightman \(1979\)](#) in which a thorough description of the physical processes between radiation and astrophysical media is presented. An important physical interaction that plays a key role in X-ray astronomy is Compton scattering ([Compton 1923](#); Nobel 1927) and in particular the opposite effect known as Inverse Compton Scattering (ICS). In this framework, a photon gains energy after interacting with a high-energy electron. When the ICS dominates as a physical process in the medium that is under study, we refer to Comptonization (multiple Compton scatterings between the photons and electrons before the photons escape the medium) where an injected radiation field transforms to a high-energy radiation field. The most straightforward way to visualize that concept is through the formula:

$$\frac{\Delta E}{E} \approx \frac{4k_B T_e - E}{m_e c^2}. \quad (1.4)$$

Here $E \ll 4k_B T_e$ for the process to be valid. For a detailed derivation and discussion of these results, see *Radiative Processes in Astrophysics* ([Rybicki and Lightman 1979](#)). In the same period a work led by [Sunyaev and Titarchuk \(1980, 1985\)](#) compiled the general processes of the Comptonization and the plasma physics along with a low energy input radiation in order to explain in detail the emergent spectral energy distribution (see also [Shapiro et al. 1976](#)). In this first attempt, they considered a spherical plasma cloud of a given radius, with electron density N_e and temperature T_e , that interacts with photons that originate from the center of the sphere. This plasma cloud should exceed by a lot the Thomson optical depth, so that the Comptonization process is efficient. The thermal equilibrium between the electrons and the photons has been already studied by [Kompaneets \(1957\)](#) and hence in their work they introduced a term that

highlights the dominance of the Comptonization quantified by the Comptonization parameter

$$y = \frac{4k_B T_e}{m_e c^2} u, \quad (1.5)$$

$$u = \sigma_T N_e c t \quad (1.6)$$

A few years later [Haardt and Maraschi \(1991, 1993\)](#) published a groundbreaking two-phase model for the X-ray emission observed in AGN, which introduced the concept of the X-ray corona, which is till now the dominant theory that explains the origin of X-rays, with the improvements that came with years of observations and simulations. In their model, the accretion flow is divided into two distinct areas. This disk is responsible for the bulk of the soft, thermal radiation (typically in the optical/UV range) produced as matter spirals in toward the black hole. It acts as a reservoir of seed photons that will later be upscattered. Situated above (and possibly below) the accretion disk, the corona is composed of a tenuous, high-temperature plasma with electron temperatures often estimated around 100 keV. In the corona, soft photons from the disk undergo inverse Compton scattering with the hot electrons, resulting in a power-law X-ray spectrum with a high-energy cutoff. This process is known as thermal Comptonization. A key aspect of the model is the energy balance between these two phases. A significant fraction of the gravitational energy released by the infalling matter is deposited in the corona, possibly via mechanisms such as magnetic reconnection, which heats the electrons. These hot electrons then upscatter the low-energy photons emitted by the disk. In turn, some of the X-rays, originating from the corona, irradiate the disk, leading to reprocessed features such as the iron $K\alpha$ fluorescence line and the Compton reflection hump. This feedback loop not only regulates the corona temperature but also shapes the emergent spectral energy distribution. (see also the review from [Mushotzky et al. 1993](#))

[Titarchuk \(1994\)](#) advanced the prior works referred to above and delivered a detailed model that is valid to explain the high-energy spectra of AGN and XRBs. The following points are discussed in detail: (a) the general formulation of the Comptonization radiative transfer problem and its reduction to the diffusion problem over energy and space; (b) the time dependence of photon escape from disk and spherical geometries; (c) the shape of the radiation spectra, taking into account relativistic corrections in the free-electron cross section and the scattering kernel; (d) the source of low-frequency photons; and (e) the recent high-energy observations and their

possible interpretation by thermal Comptonization models. This framework led to the development of models that are used to fit X-ray data such as the COMPTT model in XSPEC (Titarchuk 1994). A similar Comptonization model that treats various geometries was introduced in the same period by Poutanen and Svensson (1996) that also comes with the model COMPPS in XSPEC. A two-phase model in which the cool, optically thick accretion disk coexists with a hot, optically thin corona. In their model, the accretion disk supplies soft seed photons that are then upscattered by the energetic electrons in the corona, naturally leading to the observed X-ray continuum. This framework not only provided a clearer picture of the geometry and energy balance in these systems but also addressed important feedback mechanisms, such as pair production and energy dissipation through magnetic processes.

Over the years, extensive surveys from various X-ray observatories settled the concept of the X-ray corona, which produces a power-law spectrum with a high-energy cutoff. The photon index of the power-law spectrum is typically around 1.9, while the high-energy cutoff is around 100 keV (Marchesi et al. 2016; Ricci et al. 2017a; Del Moro et al. 2017; Tortosa et al. 2018; Baloković et al. 2020; Akylas and Georgantopoulos 2021).

The exact size of the corona is yet unknown, although various studies have suggested that it is likely to be compact, with a size on the order of a few gravitational radii. Using XMM-Newton observations of 1H 0707-495, Fabian et al. (2009) detected K and L shell iron lines for the first time, allowing them to perform a time analysis. The time lag between the emission lines and the continuum suggests that the emission comes from a region that is close to the SMBH, a few gravitational radii. Wilkins and Fabian (2013) studied the same galaxy and found that the observed lag spectrum suggests an X-ray source that extends radially to approximately $35 r_g$ and is positioned at a height of about $2 r_g$ above the accretion disc plane. Different models and geometries have been tested in order to explain the observed X-ray spectra and the time lags in a follow-up work (Wilkins et al. 2016). The best model suggests a corona that lies above the SMBH and can extend up to the inner parts of the accretion disk in a few gravitational radii.

Chartas et al. (2009) adopted a different approach to constrain the physical size of the X-ray corona. They have studied two gravitationally lensed quasars, RX J1131-1231 and HE 1104-1805, using Chandra observations and used the microlensing effect to constrain the size of the X-ray corona. The microlensing effect is a phenomenon that occurs when a compact object

(e.g., a star) passes between the observer and a background source. The gravitational field of the foreground object acts as a lens, bending the light from the background source. By combining optical and X-ray light curves, they found that the X-ray source of HE 1104-1805 must be in the order of magnitude of $\approx 6r_g$, setting a new constraint on the size of the X-ray corona.

More recently, using X-ray polarimetry from the Imaging X-ray Polarimetry Explorer (Weisskopf et al. 2022), studies have shown that the geometry of the corona can vary between sources, with no clear consensus on the exact structure of the corona. Gianolli et al. (2023) used IXPE observations of the Seyfert galaxy NGC 4151 to constrain the geometry of the corona, finding that the corona is highly unlikely to be spherical and that a slab geometry is more likely (see also, Haardt and Maraschi 1991; Merloni 2003). Ingram et al. (2023) examined the Seyfert 1 galaxy IC 4329A, and their findings indicate that despite uncertainties about the corona’s precise structure, it probably has an outflow configuration, which aligns with the observed polarization levels. Finally, Tagliacozzo et al. (2023) modeled the hot corona in MCG-05-23-16 constrained by X-ray polarimetry, using different models (spherical lamp-post, conical, slab and wedge) and proposed that the best fit comes from a conical corona and disfavor the slab geometry.

The X-ray corona plays a crucial role in the study of AGN since it is the source of the high-energy X-ray emission that is observed. As the primary region for inverse Compton scattering, the corona provides direct insight into the extreme physics occurring in the very central regions of the AGN. Despite ongoing debates regarding its precise scale, shape, and detailed geometry, whether it is more spherical, slab-like, or even conical, it is widely accepted that a compact X-ray-emitting region exists very close to the SMBH. With data from the newly launched XRISM observatory, further constraints on the size, geometry, and dynamics of the corona are anticipated, further establishing its role as a unique laboratory for extreme physics.

1.2 Commonly used X-ray models

In the previous section, we described how the evolution in the X-ray spectroscopy along with the theoretical work established that the origin of the radiation is compact and close to the

SMBH. Photons produced in the X-ray corona interact with circumnuclear material and undergo a series of interactions forming what we call the reprocessed part of the spectrum. As a result, the observed spectrum is often far from a smooth power-law. Consequently, when we analyze the spectra of AGN, we need to adopt models that, in addition to the intrinsic continuum, also take into account such interactions.

Slab geometry

One of the most widely used models for reproducing reprocessed X-ray radiation is PEXRAV⁷ (Magdziarz and Zdziarski 1995). Magdziarz and Zdziarski (1995) created a geometrical model that consists of a corona on top of a slab, which takes the place of the accretion disk. The output spectrum is the sum of the cutoff power-law⁸ and the reflection component. The coronal properties, such as the photon index Γ and the energy cutoff E_c (in keV), are free parameters in this model. The slab is characterized by the free parameter $rel_{refl}(R)$. The reflection parameter $R = \Omega/2\pi$, where Ω is the covering factor of the reflecting material. In addition, the redshift, the abundance of metals, the abundance of iron, and the angle of inclination are free parameters.

A similar model that models the reprocessed radiation is PEXMON⁹ (Nandra et al. 2007), which combines PEXRAV with a few emission lines, Fe K α , Fe K β , Ni K α along with the Fe K α Compton shoulder (e.g., Akylas and Georgantopoulos 2021). PEXMON implements the same parameters. Although PEXRAV and PEXMON are still very popular, they have some limitations. Both do not consider relativistic effects that are present close to the SMBH (e.g., Dauser et al. 2010). Moreover, the geometry is limited to a planar geometry, so they are not applicable to realistic geometries beyond the accretion disk. They also assume that the source is very close to the reflecting medium, so that the incident angle of the primary radiation is isotropically averaged. Finally, even though they provide a very good approximation of the reflection on free electrons, they suffer from inconsistencies in the implementation of iron emission lines

⁷<https://heasarc.gsfc.nasa.gov/xanadu/xspec/manual/node209.html>

⁸We refer to cut-off power-law to spectra that are reproduced by: $F = E^{-\Gamma} e^{-E/\epsilon}$, where Γ is the photon index and ϵ the folding energy. Note that the folding energy and the cutoff energy are not the same. Folding energy is a parameter in a formula that controls the exponential whereas cutoff energy is an effect that takes place where the power-law starts to decline. However, they are often used interchangeably.

⁹<https://heasarc.gsfc.nasa.gov/xanadu/xspec/manual/node208.html>

and the lack of bound-electron scatterings.

García et al. (2010, 2013) released the XILLVER¹⁰ model which is a disk-reflection model with a proper treatment of the relativistic effects that occur near strong gravitational fields. This kind of model is used to constrain the properties of the disk, including its inner radius, the degree of ionization of the gas, and the elemental abundances. Importantly, reflection models are the key to measuring black hole spin via the Fe–line method. The code XILLVER calculates the solution of the reflected intensity of the radiation field for each photon energy, position in the slab, and viewing angle. Reflection is modeled by solving radiation transfer on a 1-dimensional slab with constant density. The model includes the following free parameters: i) the photon index (Γ) of the illuminating source, ii) the energy cutoff (E_c) of the source, iii) the ionization parameter (ξ) that is related to the slab material, iv) the iron abundance with respect to the solar one (A_{Fe}) and v) the inclination angle between the disk and the observer (θ).

An improved version, named RELXIL, was introduced by García et al. (2014) which combined the reflection code XILLVER and the ray-tracing code RELLINE¹¹ (Dauser et al. 2010, 2013). The novelty of this model is that it takes into account the relativistic distortion when measuring the reflection component. This distortion enables the measurement of black hole parameters like its spin. The reflection fraction, which is the flux ratio between direct and reflected radiation, is deduced directly from the geometry and position of the primary radiation source (Dauser et al. 2014). However, the reflection fraction measured in RELXIL is not the same as the one described in PEXRAV. The reflection fraction, in PEXRAV, is defined as the ratio of the intensity of the primary source irradiating the disk and the intensity that goes directly to infinity. In the case of relativistic reflection models, such as RELXIL, the definition of the reflection fraction is different, due to relativistic light-bending (e.g., Miniutti and Fabian 2004; Fukumura and Kazanas 2007), where the location of the primary source influences the value. RELXIL consists of a family of models that implement different combination of source geometry and disk. As a result the free parameters can vary between the different implementations.

Recently, Xiang et al. (2022) released the model REXCOR, a new AGN X-ray spectral fitting

¹⁰<https://sites.srl.caltech.edu/~javier/xillver/>

¹¹<http://www.sternwarte.uni-erlangen.de/~dauser/research/relxill/index.html>

model (0.3 – 100 keV) that self-consistently combines the effects of both ionized relativistic reflection and the emission from a warm corona. In this model, they assume a lamppost X-ray source that is the main hard X-ray source, an accretion disk, and the warm corona component, which is a layer on top of the accretion disk that contributes to the soft excess (e.g., [Magdziarz et al. 1998](#); [Matt et al. 2014](#)). REXCOR implements eight parameters: black hole mass M , spin α , and accretion rate λ ; the lamppost height h and heating fraction f_X ; photon index Γ and warm corona heating fraction h_f and optical depth τ . [Xiang et al. \(2022\)](#) tested the model on joint XMM-Newton and NuSTAR monitoring campaigns of the Seyfert I galaxies HE 1143-1820 and NGC 4593.

These models represent a diverse approach to the available slab spectral models for use. Each model offers its own benefits and drawbacks, but they have consistently proven valuable to the X-ray community over the years.

Torus geometry

As discussed in the previous section, the dusty torus is crucial in obscuring AGN since the development of the unified model is mostly based on the existence of such a structure. Hence, many models have been released that consider toroidal media with various properties and limitations.

MYTORUS [Murphy and Yaqoob 2009](#) assumes an axisymmetric doughnut geometry. The model thus implements the classic orientation-dependent AGN classification paradigm. The size of the torus is determined by the ratio c/a where c is the distance from the point-like X-ray source and a is the radius of the torus cross section (e.g., [Yaqoob 2012](#)). The ratio is $c/a = 0.5$ (fixed) in the published model. The gas density is uniform throughout the torus. The equatorial column density ($N_{H,eq}$) is a variable parameter; the Line of Sight (LOS) column density ($N_{H,los}$) is derived from the ratio c/a and the inclination angle (θ_i). The MYTORUS model is valid for column densities in the range $10^{22} - 10^{25} \text{ cm}^{-2}$ and therefore provides continuous coverage from the Compton-thin to Compton-thick regimes. The model assumes that the reprocessing material is uniform, neutral, and cold. MYTorus utilizes photoelectric absorption cross sections for 30 elements as described in [Verner et al. 1996](#) and cosmic abundance based on [Anders and Grevesse 1989](#). Finally, the code implements the $K\alpha$ emission line for Fe and Ni, as well as

the Fe K β fluorescent line.

[Ikeda et al. 2009](#) introduced the ETORUS model, which assumes a smooth torus too. This model has a spherical geometry with a biconical cutout at the poles, where the cone vertices lie above/below the central point on the symmetry axis. The X-ray source is a point source in the center of the sphere. The ratio of the inner to the outer radius of the torus ($r = r_{\text{in}}/r_{\text{out}}$) is kept fixed at 0.01 in the published model. The opening angle (θ_o) is variable and, for the obscured AGN, the inclination angle (θ_i) must be ($\theta_i > \theta_o$). The model assumes that the surrounding material is neutral and cold ($T < 10^6$ K) with the metal abundance defined by [Anders and Grevesse 1989](#). Furthermore, ETORUS implements photoelectric absorption based on [Verner et al. 1996](#) and Compton scattering cross section using the Klein-Nishina formula. However, only iron fluorescent lines are included (Fe K α , Fe K β). The ETORUS model has 5 free parameters: i) the column density N_{H} in units of 10^{22} cm^{-2} , ii) the photon index of the input power law spectrum with a range of 1.5–2.5, iii) the torus opening angle, in degrees, with a range of 10–70, iv) the observing inclination angle and v) the redshift of the source. Moreover, there is a version of ETORUS that includes a high energy cutoff (E_c) parameter in keV.

RXTorus is based on the radiative transfer code REFLEX [Paltani and Ricci 2017](#). The geometry assumed is an axisymmetric doughnut. RXTorus considers a primary X-ray spectrum in the form of a power law with a photon index Γ between 1.0 and 3.0, while the maximum photon energy is set to 300 keV. Note that this corresponds to the maximum energy of the power law, and not a cutoff energy, similar to the MYTORUS model. The equatorial column density ($N_{\text{H,eq}}$) spans from 10^{22} cm^{-2} up to 10^{25} cm^{-2} . The final model consists of different Table models that assume different metallicity and dust compositions. It comes in several variations based on the population of photons collected (i.e. scattered, fluorescent etc.)

[Baloković et al. 2018](#) using the Monte Carlo radiative transfer code BORUS, released the table model BORUS02. BORUS02 represents only the reprocessed spectral component (separated from the line-of-sight component), while featuring both the average column density and the covering factor as free parameters. The torus covering factor, as seen from the X-ray source, is simply related to the half opening angle of the torus, θ_{tor} , as $C_{\text{tor}} = \cos \theta_{\text{tor}}$. The BORUS02 has the same geometry parametrization as adopted in the BNTORUS model introduced by [Bright-](#)

man and Nandra 2011.

Recently, more complicated models have been released that include clumpy torus geometries. Tanimoto et al. 2019 introduced the XCLUMPY torus model which is an X-ray extension of the CLUMPY infrared torus model Nenkova et al. 2008a. The torus is not a smooth medium. On the contrary, it is composed of many clumps randomly distributed following a given number density function. For simplicity, each clump is a sphere with a radius of R_{clump} and has a uniform hydrogen number density n_{H} . For the clumps, a power-law distribution in the radial direction between inner and outer radii is assumed, and a normal distribution in the elevation direction. To summarize, XCLUMPY model has eight independent parameters that define the torus properties: (1) inner radius of the torus (r_{in}), (2) outer radius of the torus (r_{out}), (3) radius of each clump (R_{clump}), (4) number of clumps along the equatorial plane ($N_{\text{clump}}^{\text{Eq}}$), (5) index of the radial density profile (q), (6) torus angular width (σ), (7) hydrogen column density along the equatorial plane (N_{H}^{Eq}), and (8) the inclination angle (i , the polar angle of the line-of-sight).

Finally, Buchner et al. 2019 released the UxClumpy (Unified X-ray Clumpy model), which is also based on the CLUMPY infrared model, featuring the same toroidal geometry. The free parameters of the model are related to 1) the source: the photon index and energy cutoff (E_{c}), 2) the obscurer: i) line-of-sight column density (N_{H}), ii) cloud dispersion (σ), iii) covering factor (C) and iv) viewing angle (θ).

The models described above are just a few examples of what is used in the literature. In combination with the slab models described in the previous paragraph, they have been the Swiss knife for X-ray spectral modeling for many years. However, an important drawback is the fact that individual models do not feature any kind of interaction or connection between them. In simpler words, the photons that might originate from the disk are not aware of the torus existence and therefore do not interact with it. Similarly, the torus will work mostly as an obscurer to some abstract input radiation. The reality dictates that there is a continuous interplay between the radiation and the circumnuclear material. In the current work, we are motivated by the aforementioned limitation and build models that are fully self-consistent systems where all the components are in constant interplay via the X-ray photons.

1.3 The ray-tracing platform *RefleX*

REFLEX is a ray-tracing code developed by [Paltani and Ricci \(2017\)](#) that is focused on the X-ray band and the reflection of the X-ray photons onto the surrounding material. Throughout

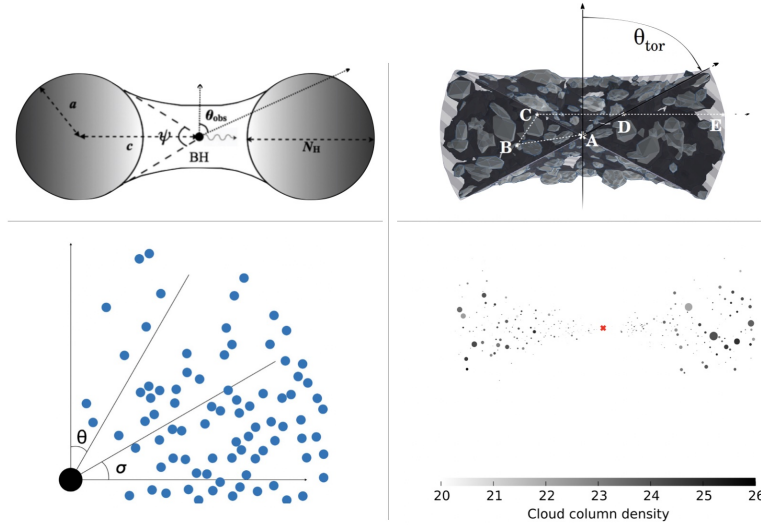


Figure 1.12: Schematics of different models used in the literature. *Top left*: A cross-section of the toroidal geometry used in the MYtorus model. The half opening angle is given by $\frac{\pi-\psi}{2}$ and the inclination angle by θ_{obs} . The equatorial column density N_{H} is defined by the diameter of the tube. Figure from [Murphy and Yaqoob \(2009\)](#). *Top right*: Cross-section of the approximately toroidal geometry adopted for borus02 model. The half opening angle of the torus, θ_{tor} (or, equivalently, the covering factor, $C_{\text{tor}} = \cos(\theta_{\text{tor}})$) is a free parameter of the model. The white asterisk in the middle (point A) represents the X-ray source. Figure from [Baloković et al. \(2018\)](#). *Bottom left*: Cross-section view of the torus of the XCLUMPY model. It is assumed a power-law distribution of the clumps in the radial direction and a normal distribution in the elevation direction. Figure from [Tanimoto et al. \(2019\)](#). *Bottom right*: Cross-section of clumpy torus model used in UXCLUMPY. The geometry is defined in the vertical axis by the parameter σ , which controls the Gaussian distribution away from the equatorial plane. The red cross indicates the central point source. The clouds vary in size and column density (darkness). Figure from [Buchner et al. \(2019\)](#).

the doctorate program we incorporate REFLEX since it provides tools to the user that can make the development of spectral models flexible.

The production of spectral models should comply with the results you want to achieve. In our case, what comes first is the energy band that we are interested in, which is the X-ray band from 0.3 keV to a few hundreds of keV. Next, comes the flexibility to build distinct models using various geometries for each case. The platform we use utilizes all the major physical processes found in the objects under study and therefore generates realistic spectra, which is the goal of this work. Finally, user-friendliness and adaptability with respect to scripting and computational expenses were also critical factors in its selection.

As a ray-tracing code it generates single photons with specific energies, based on a distribution selected by the user. The photons traveling inside the simulation WORLD and when they intercept the physical object, the code using a Monte Carlo method calculates the event based on the given cross sections that have been precalculated accordingly. After the event, the same process is executed until the outcome of the calculations enables the photon to exit that object. WORLD is a characteristic object in the code that sets the limit of the simulation space, where the photons are collected. All energies and directions are carefully treated and stored in the lifetime "memory" of the photon. This procedure repeats for all the photons until all are collected. REFLEX implements the full Klein-Nishina relativistic differential cross section to treat the interactions between the photons and free electrons, as well as the necessary corrections for bound electrons. Rayleigh coherent scattering on atoms is also included. An important aspect of ray-tracing codes is the proper implementation of photoelectric absorption and consequently recombination, which leads to emission lines. REFLEX includes the full photoelectric cross sections for 30 elements (only neutral atoms) and the Auger effect, which is the emission of a secondary electron after the photoelectric absorption of a photon (for more details, see [Paltani and Ricci 2017](#)). In the updated version of the code ([Ricci and Paltani 2023](#)), REFLEX 3.0, interactions between photons and dust grains have been implemented, which is crucial for the study of the dusty media around AGN.

Chapter 2

Realistic X-ray spectral models with RefleX

This chapter introduces the development of two new X-ray spectral models, RXTOPo and RXAGN1, which are designed with the aim of providing realistic circumnuclear material. The models were developed using the ray-tracing code REFLEX, which was presented in Section 1.3. The RXTOPo model includes a torus and a polar hollow cone, while the RXAGN1 model extends the RXTOPo model by including an accretion disk and a broad line region. The models are designed to reproduce the X-ray spectra of AGN, taking into account all the different structures present in these systems. Next, we test them by fitting the combined *XMM-Newton* and *NuSTAR* spectra of NGC 424, an obscured AGN in which the X-ray emission is dominated by reflection features. The models are introduced to the public via a paper that has been recently submitted to the *Astrophysical Journal*. The models will be publicly available through the REFLEX website¹.

2.1 Introduction

In the previous chapters, we have presented a series of different configurations of the material that surrounds the SMBH that lurks at the very center of AGN. This material varies in terms of composition as well as geometrical characteristics. In Section 1.2 we illustrated the impact

¹<https://www.astro.unige.ch/reflex/>

of these media on X-ray spectra, since they reprocess the intrinsic continuum radiation. In the models mentioned, the common factor is the simplified geometries used. Despite the fact that each one can represent with significant accuracy specific gas distributions overall deviate from what modern AGN models suggest.

Although we do not yet have a complete understanding of the immediate environments of SMBHs, a widely accepted theory suggests that a thick torus of dust and gas obscures the central region (see Section 1.1.5. In most AGN ($\sim 60 - 70\%$) in the local Universe the X-ray source is obscured (Ricci et al. 2015). The dusty torus is expected to absorb a significant amount of the disk emission and re-emit it at infrared wavelengths (e.g., Rowan-Robinson 1995, 1998; Stalevski et al. 2016). The accretion disk and the dusty torus are expected to be connected through the broad line region (BLR), where broad emission lines are produced by the high velocity of the gas ($> 2000 \text{ km s}^{-1}$; e.g., Peterson et al. 1991; 1993; 2004, Kaspi et al. 2000; Goad et al. 2012; GRAVITY Collaboration et al. 2020a, 2024b). In very bright and nearby AGN, such as the Circinus galaxy and NGC 1068, mid-infrared observations have revealed the presence of dust extending in the polar direction (e.g., Hönig et al. 2013; López-Gonzaga et al. 2014; Asmus et al. 2016; Stalevski et al. 2017). This extended emission could be associated with winds originating from the central region of the AGN, driven by the radiation pressure on the dust (e.g. Fabian et al. 2006; Hönig and Beckert 2007; Venanzi et al. 2020), in agreement with X-ray observations (Ricci et al. 2017d, 2022; Laloux et al. 2024).

To accurately reproduce the reprocessed X-ray radiation observed in AGN, it is essential to consider all the different aforementioned structures present in AGN, such as the accretion disk, broad line region, torus, and polar dust. X-ray photons are expected to interact with all these components; thus, simplified approaches, where each component is separate, have limitations that can affect the final values of the properties. In other words, each component is responsible for reproducing a specific part of the spectrum, whereas the reality is different, and there is a constant interplay between them and the photons.

In this work, we develop two new complex models. The first model, RXTOPO, includes a polar hollow cone (representing the polar dusty gas) and a torus. The second model, RX-AGN1 is an extension of RXTOPO and includes, besides the torus and polar dust, an accretion disk and a broad line region. To build the models we use REFLEX (for details Section 1.3)

In Section 2.2.1 and Section 2.2.2 we introduce the two new spectral models, including all the details necessary for the reader to understand how they were built, as well as their physical motivation. Next in Section 2.3 we present the format of the models along with the different available variations of each model in terms of the physical processes recorded in order to generate them. We demonstrate the capabilities of these two new models by fitting the combined *XMM-Newton* and *NuSTAR* spectra of NGC 424, a heavily obscured AGN in which the X-ray emission is dominated by reflection features. Finally, we present our summary and conclusions in Section 2.4.

2.2 Simulation setup

2.2.1 The RXTOPo model

Paltani and Ricci (2017) along with the release of the REFLEX code, published the table model RXTORUS, which implements a toroidal reprocessing medium and the X-ray source. The free parameters of this model are the torus column density and covering factor, as well as the photon index of the primary X-ray continuum. The covering factor is defined as the ratio r/R between the inner cutout radius of the doughnut r and the distance from the center of the simulation R , i.e. the SMBH. The torus is expected to be composed of a mixture of gas and dust, and to reside outside the sublimation zone (e.g., Mor et al. 2009; GRAVITY Collaboration et al. 2020b). Therefore, more recently an updated version of this toroidal model, including scattering and absorption associated with dust grains, RXTORUSD (Ricci and Paltani 2023), was released.

We introduce here a new model, RXTOPo, which can be considered as an extension of RXTORUSD. This model includes, in addition to the dusty torus, a polar dusty cone perpendicular to the accretion disk. In Fig. 2.1 a cartoon of the model is shown, featuring all the components mentioned above. The RXTOPo model has five free parameters (see Table 2.1): i) the photon index (Γ) of the primary power-law continuum, which varies from 1.6 to 2.4; ii) the observing angle of the system (θ_o), which extends from zero degrees (face-on view) to 90 degrees (edge-on view); iii) the equatorial column density (N_H^{tor}) and iv) the covering factor (CF^{tor}) of the dusty torus (details in Section 2.2.1); v) the column density of the polar

hollow cone (N_H^{pol}), which is calculated along the inner surface of the hollow cone (details in Section 2.2.1). In the following, we describe in detail how the different components used in the models were developed.

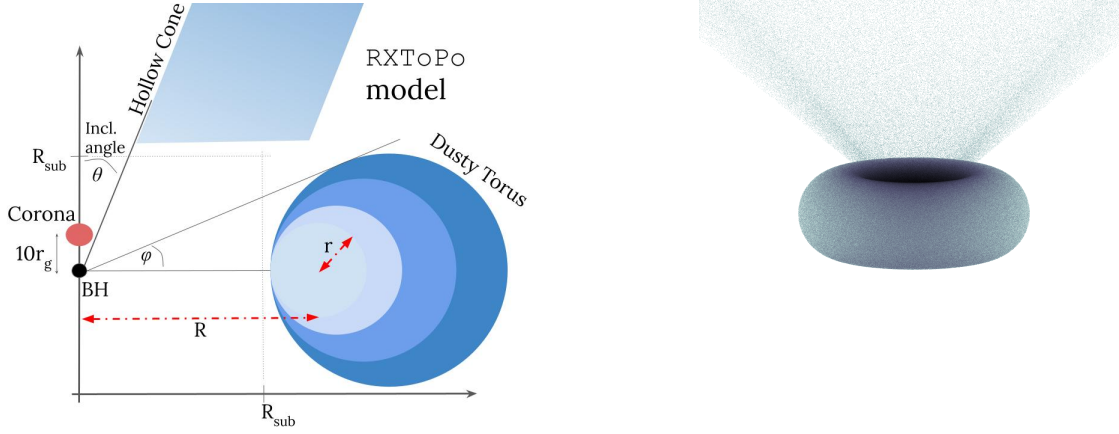


Figure 2.1: (Left) A visual illustration of the configuration of the RXTOPo model. In the center of the system is the SMBH with the corona placed on top of it. The torus can be found after the sublimation zone with a variable size. Perpendicular to the plane of the torus is the hollow polar cone. The dash-dotted line (red) depicts the R and r that are used to calculate the covering factor of the torus. The components are not scaled. The angle θ is the observing angle of the system. ϕ is the opening angle of the torus. (Right) An image generated using REFLEX showing a torus with $CF^{\text{tor}} = 0.6$ and the polar hollow cone with 10° angular width.

The X-ray source

Our model uses as an X-ray source a corona-like component by adopting, for simplicity, the lamp-post scenario (e.g., Fabian et al. 2009; Emmanoulopoulos et al. 2014; Uttley et al. 2014). To implement such a component we used a sphere that is placed $10r_g^2$ above the SMBH (i.e. the center of the simulation box since there is no physical black hole in the simulation). A spherical or point source placed at the very center of the simulation would have been fully obscured by the optically thick accretion disk included in our simulation, and hence we decided to place it on top of the SMBH. Moreover, the system is observed from 0° to 90° from the

² r_g is the gravitational radius: $r_g = 2GM/c^2$, where G is the gravitational constant, M_{BH} is the black hole mass, and c is the speed of light.

zenith to the plane of the SMBH and therefore we included one X-ray source at $+10r_g$ without physical motivation for the absence of an X-ray source at $-10r_g$. The spherical corona is assumed to have a radius of $6r_g$ (e.g., Chartas et al. 2009; De Marco et al. 2013). To estimate the physical distance, we considered the black hole mass of the Circinus galaxy: $\log(M_{\text{BH}}/M_{\odot}) = 6.23$ (Koss et al. 2017). The spatial parameters of the X-ray source are fixed throughout all of our simulations.

The next step is to define the spectral properties of the X-ray source. The photons are generated following a cutoff power law distribution (e.g., Zdziarski et al. 1996; Dadina 2008; Ricci et al. 2017a), following the `cutoffpl`³ model in XSPEC. The simulated photons cover a wide energy range from 0.3 to 300 keV. Yet, when collected by REFLEX they are divided into two separate files with different binning. From 0.3 to 10 keV the original simulation output has 2 eV binning resolution, a decision motivated by the fact that the XRISM/*Resolve* microcalorimeter (XRISM Science Team 2020) delivers ≤ 7 eV spectral resolution in the energy band 0.3 – 13 keV. Such high spectral resolution comes with computational cost which is translated into noisy spectra. To accommodate that issue, we decided to rebin by a factor of 10 the spectra from 0.3 to 10 keV, except for the energy regions of Fe K α , Fe K β (including the iron edge) and Ni K α where the binning remains to 2 eV. For the energies above 10 keV we applied a logarithmic binning with a step size of 0.01. The cutoff energy of the spectrum is fixed to 200 keV, corresponding to the median value of nearby AGN (Ricci et al. 2018). The photon index Γ varies from 1.6 to 2.4, covering the range typically observed in AGN (e.g., Piconcelli et al. 2005; Ricci et al. 2017a). In Table 2.1 we summarize the properties of the X-ray source.

The dusty torus

The primary medium responsible for obscuring the central source is a structure that resides after the sublimation zone, usually referred to as "the torus" (Krolik and Begelman 1988; Jaffe et al. 2004; Mor et al. 2009; Davies et al. 2015; Ramos Almeida and Ricci 2017). Our torus starts at the sublimation radius, which was calculated for a given bolometric luminosity (L_{bol})

³<https://heasarc.gsfc.nasa.gov/xanadu/xspec/manual/node161.html>

using the relation reported by [Mor et al. \(2009\)](#):

$$R_{\text{sub}} = 1.3 L_{46}^{0.5} \times \left(\frac{1500\text{K}}{T_{\text{sub}}} \right)^{2.6} \text{ pc} \quad (2.1)$$

where R_{sub} and T_{sub} are the sublimation radius and temperature, respectively, while $L_{46} = L_{\text{bol}}/10^{46} \text{ erg s}^{-1}$. We adopted the 2–10 keV luminosity of the Circinus galaxy ($L_{2-10} = 3 \times 10^{42} \text{ erg s}^{-1}$, [Arévalo et al. 2014](#)), and converted the X-ray luminosity to bolometric using as bolometric correction $\kappa = 20$ ([Vasudevan and Fabian 2009](#)).

The physical parameters of the torus are set so that the material is neutral and dusty, while the molecular hydrogen fraction is set to $H_2 = 0.3$ (e.g., [Wilms et al. 2000](#); [Wada et al. 2009](#)). For the torus, we assumed the 1pgs metal abundance ([Lodders et al. 2009](#)), metallicity $Z = 1$ and an iron dust depletion of 1.0, which means that all Fe atoms are found in dust grains (see [Ricci and Paltani 2023](#) for details). The amount of gas and dust inside the torus is controlled by the volumetric density of the object. To determine the correct volumetric density of the torus, we divide the equatorial column density, a free parameter, by the diameter of the cross section of the torus. This calculation assigns the correct volumetric density in the model via the free parameter $N_{\text{H}}^{\text{tor}}$. The parameter range is $\log(N_{\text{H}}^{\text{tor}}/\text{cm}^{-2}) = 22 - 25.5$. We binned the values of this parameter as follows: from $\log(N_{\text{H}}^{\text{tor}}/\text{cm}^{-2}) = 22$ to 23.3 we considered bins of $\Delta \log(N_{\text{H}}^{\text{tor}}/\text{cm}^{-2}) = 0.3$, followed by bins of $\Delta \log(N_{\text{H}}^{\text{tor}}/\text{cm}^{-2}) = 0.2$. These bins have been selected considering the total size of the model grid and the computational cost.

The size of the torus in the model is regulated by the ratio of the inner radius (r) to the distance from the SMBH (R). This ratio is also the $\sin(\phi) = r/R$ which is the angle that corresponds to the covering factor (Fig. 2.1). Hence, we introduce the parameter $CF^{\text{tor}} = \sin(\phi) = r/R$, which varies from 0.1 to 0.9 with a step size of 0.1. The maximum value of 0.9 translates into an opening angle of the torus of 65° . It should be emphasized that the total sky coverage of the obscuring material may be larger than the covering factor of the torus, as the polar component also contributes to it. (see, Section 2.2.1). The properties of the torus adopted in our simulations can be found in Table 2.1, while the column density profile of this component is shown in Fig. 2.2 for two different covering factors.

The polar cone

Infrared observations of local AGN suggest the presence of an extended region that can reach hundreds of parsecs, composed of warm dust (e.g. [Stalevski et al. 2017](#); [Asmus 2019](#); [Alonso-Herrero et al. 2021](#)). In the RXTOPo model, we implement this dusty structure by adopting a hollow cone geometry, similar to that which has been shown to effectively reproduce the IR emission of the Circinus galaxy ([Stalevski et al. 2017, 2019](#)). In Fig. 2.1 we illustrate the cone component, while the column density profile of the RXTOPo model is shown in Fig. 2.2. The hollow cone has the angular width set to 10° . The opening angle of the cone, or in other words the angle at which the cone starts intercepting the X-ray source, is controlled by the torus. In our model, the torus collimates the polar cone, since this structure is associated to the material that has been expelled from the dusty torus (e.g., [Venanzi et al. 2020](#)). We use the opening angle of the torus (ϕ , see for details Section 2.2.1), and we set the cone to have a maximum angle $\xi_{\max}^{\text{pol}} = \phi + 1^\circ$, to ensure that the two components do not overlap. The opening angle of the cone is therefore $\xi_0^{\text{pol}} = \xi_{\max}^{\text{pol}} + 10^\circ$.

The material in this component is set to be neutral with metallicity $Z = 1$ and molecular hydrogen fraction $H_2 = 0.3$, similar to the torus, since they reside both at similar distances from the SMBH. Similarly to the torus, the metal abundance used is 1pgs ([Lodders et al. 2009](#)). The polar cone is placed above the sublimation radius since it is assumed to be dusty. Therefore, we set the base of the geometrical object at R_{sub} (see equation 2.1), as it was done for the torus. The material that eventually settles in the polar cone originates from inner parts of the system and therefore it is natural to assume that there should be another "component" that lies between the innermost regions and the polar cone. Yet, the main motivation for the polar cone is to account for the extended emission observed in the IR, and therefore we decided to include it in the model. Moreover, the X-ray spectrum is affected by the column density across the line-of-sight and hence the free parameter $N_{\text{H}}^{\text{pol}}$ accommodates any additional neutral material that could be present in the system. Ionized winds are present in many cases but they are not part of this study and therefore ionized material and high velocity material will be included in future versions of the models when they are available in REFLEX (e.g., [Psaradaki et al. 2024](#)). The dust depletion is also set to 1.0 (see Section 2.2.1 and [Ricci and Paltani 2023](#)), since the

dust grains are formed rapidly after passing the sublimation zone due to the outflowing material (e.g., [Mehdipour and Costantini 2018](#)). The outer boundary of the conical structure is set to 40 pc. While there is no clear ending point to the upper boundary of the cone and the material is expected to be distributed even further away (e.g., [Asmus 2019](#) and more recently [Haidar et al. 2024](#)), our motivation is to include the most dense circumnuclear region which can influence the X-ray photon field that emerges from the corona. The column density of the hollow cone is a free parameter and it is calculated along the innermost surface of the cone. It spans a range of $\log(N_{\text{H}}^{\text{pol}}/\text{cm}^{-2}) = 22.0 - 24.0$ (e.g., [Asmus 2019](#); [Venanzi et al. 2020](#)), with a step size of $\Delta\log(N_{\text{H}}^{\text{pol}}/\text{cm}^{-2}) = 0.25$. In [Table 2.1](#) we report the properties of the cone and in [Fig. 2.2](#) you can see the effect of the polar hollow cone on the line-of-sight column density.

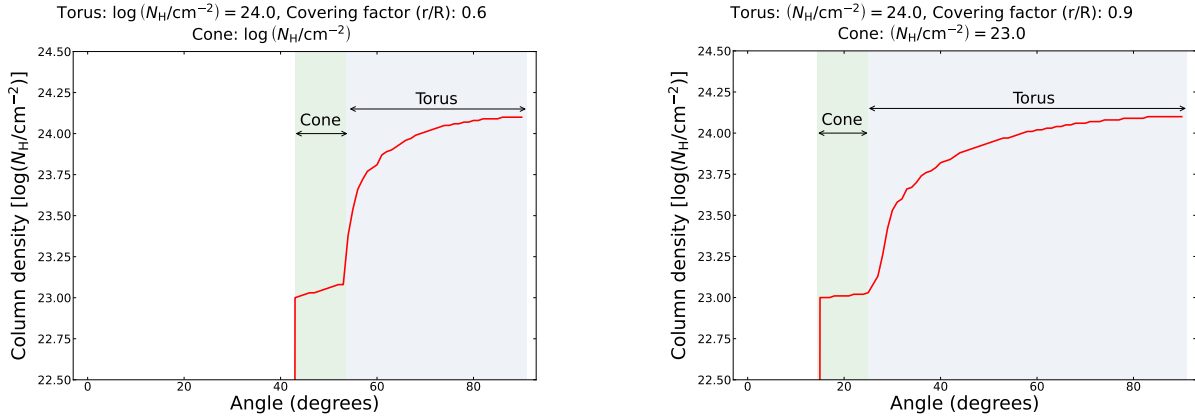


Figure 2.2: Two examples of column density profile for the RXTOPo model, considering two different torus configurations. In both panels we show the line-of-sight column density varies for different angles. The shaded areas that are also noted by the arrows mark the angle range in which the cone or torus intercept the photons that originate from the center. In the left panel we considered a torus with $CF^{\text{tor}} = (r/R) = 0.6$, whereas the right panel shows a torus with $CF^{\text{tor}} = 0.9$.

2.2.2 The RXagn1 model

The second new model presented here is RXAGN1, an extension of the RXTOPo model that incorporates additional components to account for all relevant AGN structures. In addition to the torus (§2.2.1) and the polar medium (§2.2.1), RXAGN1 includes the accretion disk (§2.2.2)

Table 2.1: Properties of the components used in the RXTOPo model. The free parameters of the model are shown in boldface. Note that column densities are expressed in units of $[\log (N_{\text{H}}/\text{cm}^{-2})]$. More details are included in Section 2.2.1

X-ray source	
REFLEX element	sphere
Γ	1.6 - 2.4
Ec [keV]	200
Band	0.3 - 300 keV
Binning (0.3 - 10 keV)	linear $\Delta E = 20$ eV
Binning (10 - 300 keV)	$\Delta \log(E/\text{eV}) = 0.01$
Torus	
REFLEX element	torus
State	neutral
H ₂ , Z	0.3, 1
Dust	1.0
Column Density	22.0 - 25.5
$CF^{\text{tor}}(r/R)$	0.1 - 0.9
Hollow Cone	
REFLEX element	Cone
State	neutral
H ₂ , Z	0.4, 1
Dust	1.0
Angle (width)	10°
Column Density	22.0 - 24.0

and the broad line region (§2.2.2), both of which are well-established components of the circumnuclear environments around SMBHs (e.g., Netzer 2015).

The RXAGN1 model has the same configuration for parameters shared with RXTOPo. In other words, the torus has as free parameters the column density ($N_{\text{H}}^{\text{tor}}$) and the covering factor (CF^{tor}). However, we decided to set a minimum covering factor of the torus $CF^{\text{tor}} = 0.2$. The motivation behind this change in the range of the CF^{tor} , is the presence of the broad line region (BLR). Even though the two elements (BLR, Torus) are not linked within our models we consider unphysical the combination of a very small torus along with a bigger BLR. Hence, the range of the covering factor of the torus is $CF^{\text{tor}} = 0.2 - 0.9$. In the case of the polar hollow cone the column density across the inner surface is a free parameter as presented in §2.2.1. Finally, similar to the RXTOPo model the photon index and the observing angle are free to vary (see §2.2.1 for details). The two new elements included, BLR and accretion disk, have their parameters fixed and are summarized in Table 2.2. The RXAGN1 model is illustrated in Fig. 2.3. To demonstrate the influence of the BLR, Fig. 2.4 shows examples of the line-of-sight column density for two different tori configurations.

The accretion disk

The accretion disk (AD) is the structure that is expected to "feed" the SMBH, and it is widely thought to be responsible for the strong nuclear emission observed in the optical and UV. To model the AD we adopted the Shakura-Sunyaev (SS73) model (Shakura and Sunyaev 1973), which considers a geometrically-thin, optically-thick accretion disk. We set the disk to start at $10r_{\text{g}}$ from the center and extend up to $1000r_{\text{g}}$, to be consistent with recent studies of optical variability (e.g. McHardy et al. 2023). We set the metallicity to unity, and used the `lpgs` abundance for consistency with the other objects. Due to the high temperatures in the disk, the hydrogen and helium are fully ionized and the medium dust-free. Finally the volumetric density is fixed to $n_{\text{H}} = 10^{12} \text{ cm}^{-3}$ (e.g., García et al. 2013). The current version of our model does not incorporate any general relativity effect. In Table 2.2 we summarize the properties of the disk.

The broad line region

The second additional object included in the RXAGN1 model is the broad line region (BLR). The BLR is the region where broad emission lines are produced, which implies the presence of gas that revolves at velocities that can reach up to a few hundreds thousands of km/s. The current version of RXAGN1 model does not include any velocity broadening associated with the motion of the BLR clouds. It will be implemented in a future version of REFLEX. Yet, the BLR can provide additional obscuration for high inclination angles (see Fig. 2.4). We assume that the BLR extends from the end of the AD up to the sublimation zone where the torus starts. To model the BLR we used a flare disk model (e.g., [Gravity Collaboration et al. 2018, 2020a](#)). To develop this model, we used the annulus geometry provided by REFLEX. A series of 30 consecutive annuli was generated. These annuli vary in width (i.e. inner and outer radius from the center of the simulation) and height. Using this method, we develop a model for the BLR, where its center is associated with the luminosity-weighted distance as described by [Kaspi et al. \(2005\)](#). In our model, the height of the BLR annuli increases logarithmically. The volumetric density spans from $n_{\text{H}} = 10^9 \text{ cm}^{-3}$ to 10^6 cm^{-3} , which is consistent with a medium that connects the denser disk with the lower density torus (e.g., [Ferland et al. 1992](#); [Goad et al. 2012](#)). In Fig. 2.4 the column density profile of RXAGN1 model is illustrated including the BLR. In our simulations, the BLR is dust-free since it ends at the sublimation zone. The gas is assumed to be neutral and the molecular hydrogen fraction is set to 20%. We use the `lpgs` metal abundance, and the metallicity is fixed to unity. In Table 2.2 we summarize the properties of the BLR.

2.3 The models

2.3.1 The spectral models

As described in Section 1.3 REFLEX gives the user the freedom to select the photons collected according to the type of interactions they have undergone. For example, continuum photons can be distinguished from scattered or fluorescent photons. We have used this option when transforming the simulation output into spectral model files, providing four different variations

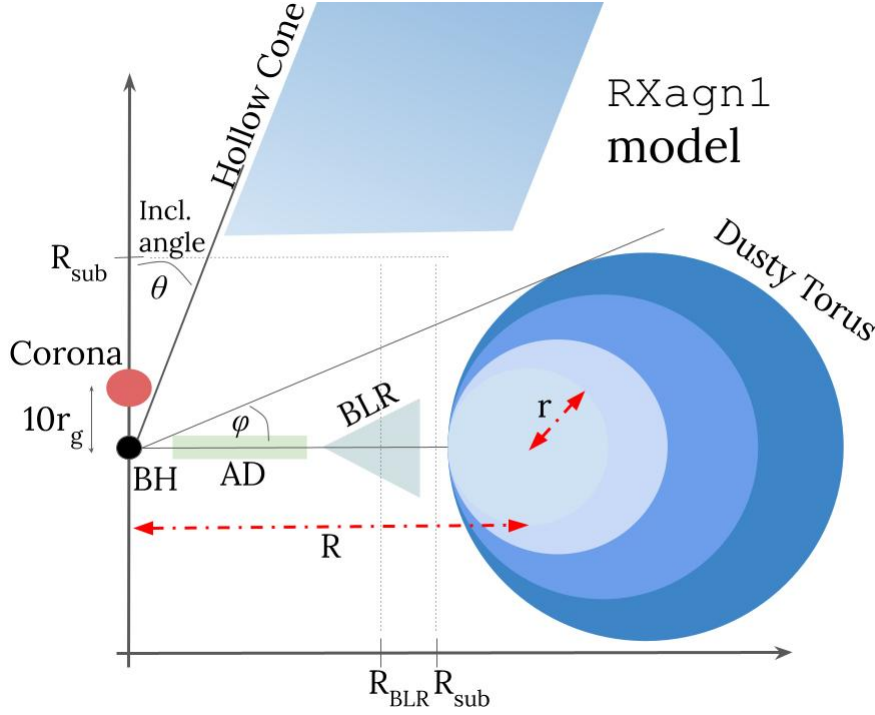


Figure 2.3: Cartoon illustrating the configuration of the RXAGN1 model. This model is an extension of the RXTOP0 model, with the addition of an accretion disk (AD) and a broad line region (BLR). The objects are not scaled. The angle θ is the observing angle of the system. ϕ is the opening angle of the torus.

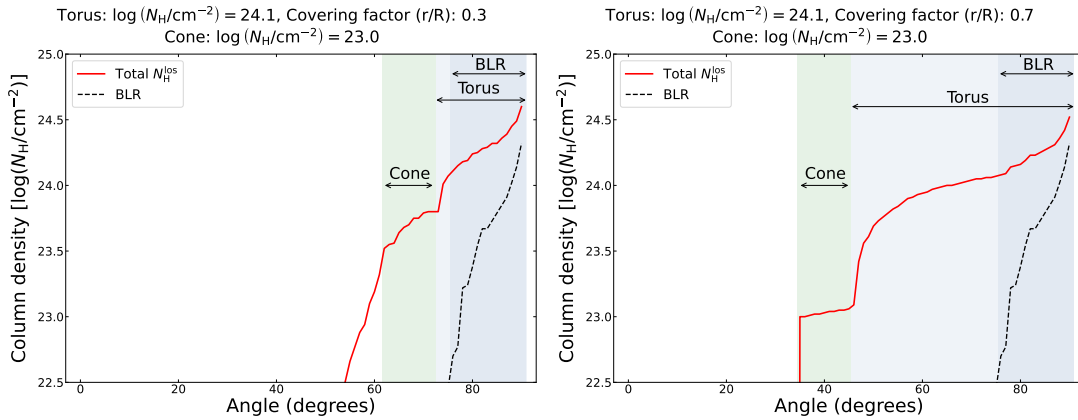


Figure 2.4: The line-of-sight density profile of the RXAGN1 model. The solid line represents the total line-of-sight column density whereas the dashed line illustrates the contribution of the broad line region (BLR). Left: The density profile of the RXAGN1 model for $CF^{\text{tor}} = 0.3$. Right: The density profile of a larger torus with $CF^{\text{tor}} = 0.7$.

Table 2.2: The properties of the extra components used in the RXAGN1 model. All the parameters of the accretion disk and BLR are fixed. The RXAGN1 model includes the components of Table 2.1 too.

Accretion disk	
REFLEX element	disk
State	H,He ionized
H_2	0
Z	1
Volumetric density (n_H)	10^{12} cm^{-3}
Dust	0
Broad line region	
REFLEX element	complex of annuli
State	neutral
H_2	0.2
Z	1
Volumetric density (n_H)	$10^9 - 10^6 \text{ cm}^{-3}$
Dust	0

of both the RXTOPo and RXAGN1 model (see details about the simulations in Section 2.2). The first variation, which is labeled as "INT" consists of all the interacting photons (including fluorescent photons) and excludes the continuum photons. The second variation is labeled as "SCAT" and has been developed by collecting all the scattered photons excluding fluorescent photons (i.e., the "INT" - emission lines). The third variation consists of only fluorescent photons ("FLUO"). The next option available is a spectral model that consists of all the collected photons. This model includes the continuum photons that originate directly from the source, as well as the previously described "INT" photons. We note this model with the suffix "ALL". Finally, there is a transmitted component ("TRNS") which consists of all the photons that did not interact with the material, whatsoever. All the different variations described above are illustrated in Fig. 2.5

These four variations of the models provide users with the flexibility to select the appropriate one based on the source being studied. As a result, these tables can be used in conjunction with other phenomenological or physical models to accommodate the various combinations needed. In Fig. 2.6 we present a few examples of the newly developed RXTOPo and RXAGN1. In the figures, we have selected two different observing angles, 45° and 85° , as well as two torus column densities $\log(N_{\text{H}}^{\text{tor}}/\text{cm}^{-2}) = 24.0, 25.0$. The photon index is $\Gamma = 1.8$, the covering factor of the torus is $CF^{\text{tor}} = 0.6$, while the polar cone has column density $\log(N_{\text{H}}^{\text{pol}}/\text{cm}^{-2}) = 22.4$. On the top panels where the observing angle is does not intercept the BLR the two modeled spectra are similar, yet in the bottom panels where the BLR is intercepting the line of sight the RXAGN1 model shows higher absorption.

2.3.2 Application on NGC 424

Having developed these two new models, RXTOPo and RXAGN1, we are interested in applying both of them to test their capabilities. We applied both models to NGC 424, one of the closest Compton-thick (CT) AGN detected by Swift/BAT (Ricci et al. 2015), at a luminosity distance of $d_L = 45.6 \text{ Mpc}$ ($z = 0.011761$). NGC 424 was confirmed to be CT by Matt et al. 2000 (Tololo 0109–383) using *BeppoSAX* observations. They found that the central source is obscured by cold material that exhibits column density of $2 \times 10^{24} \text{ cm}^{-2}$. Later, Marin-

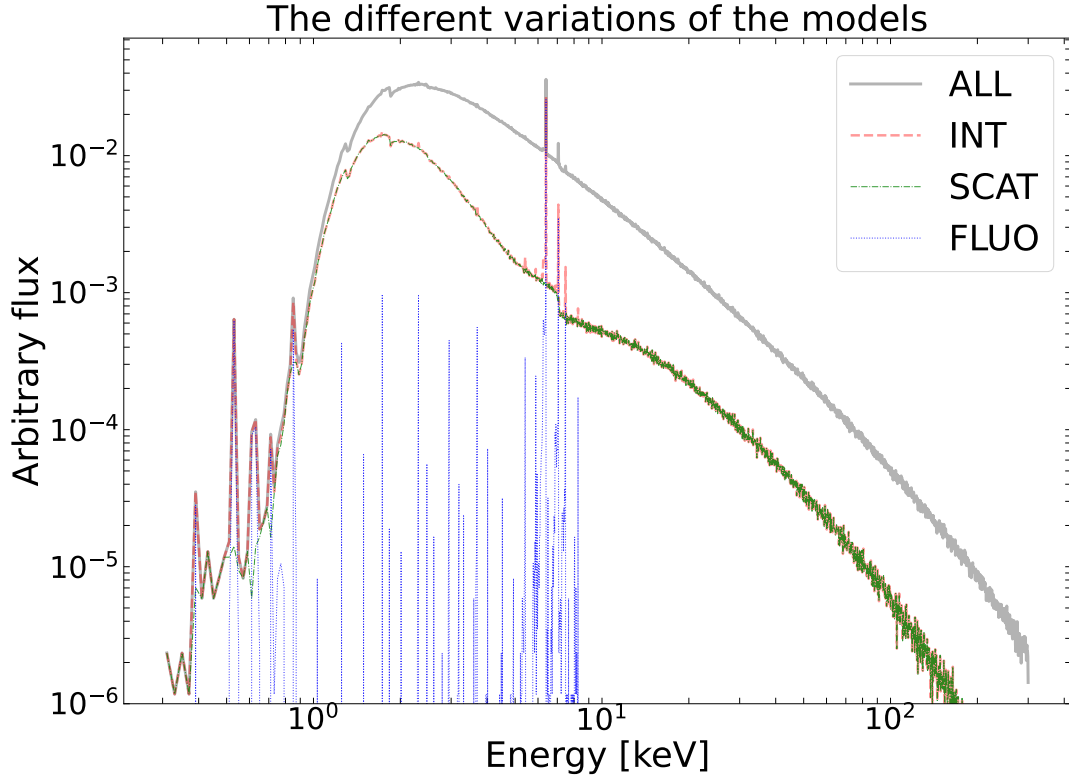


Figure 2.5: Different variations available for the RXTOPo and RXAGN1 models as described in Section 2.3.1. The different lines represent the different interactions photons undergo: ALL when all the photons are collected (grey solid line), INT for the photons that interact with the material (either by scattering or fluorescence; dashed red line), SCAT (dashed green line) and FLUO (solid blue line) for the photons that undergo scattering and fluorescence, respectively. Here we illustrate the RXTOPo model with the following parameters: $\text{Torus } \log(N_{\text{H}}^{\text{tor}}/\text{cm}^{-2}) = 24.0$, $CF^{\text{tor}} = 0.6$ and $\text{Cone } \log(N_{\text{H}}^{\text{pol}}/\text{cm}^{-2}) = 22.4$.

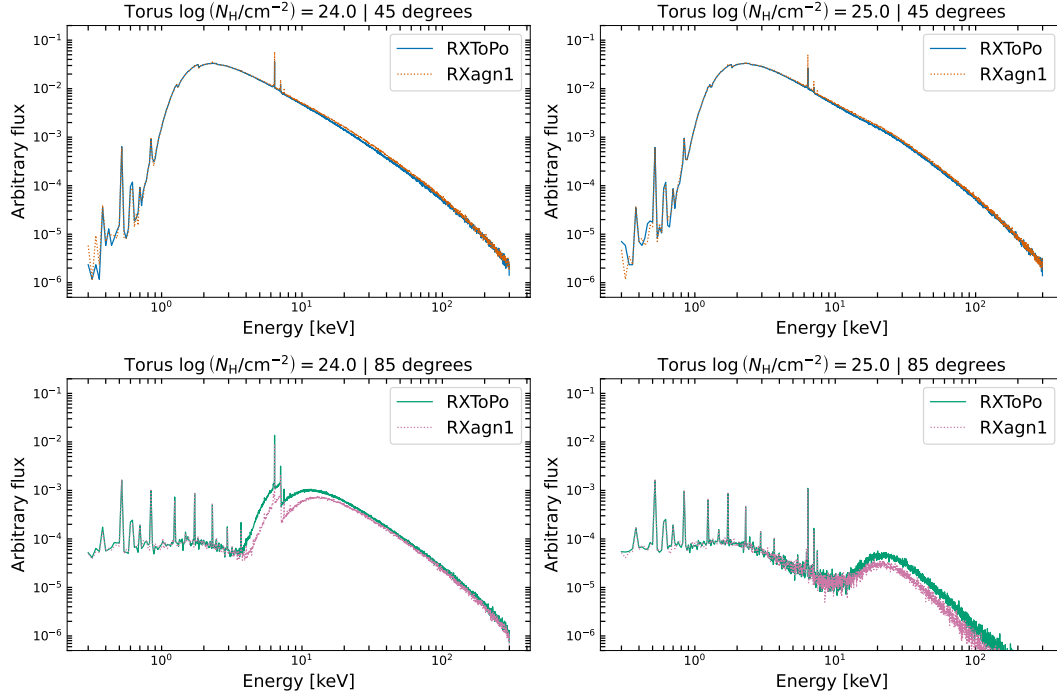


Figure 2.6: The four panels illustrate a few examples of the simulated spectra. In every panel are presented both the RXTOPo and RXAGN1 model. The top row shows two different versions of the torus with $\log(N_{\text{H}}^{\text{tor}}/\text{cm}^{-2}) = 24.0$ (left), 25.0 (right), $CF^{\text{tor}} = 0.6$ and Cone $\log(N_{\text{H}}^{\text{pol}}/\text{cm}^{-2}) = 22.4$ observed at 45 degrees. The bottom row is the same configuration but observed at 85 degrees.

ucci et al. 2011 studied thoroughly the same source using *XMM-Newton* RGS and EPIC-pn and found that the soft part (< 2 keV) of the spectrum shows several emission lines from ionized material, and the harder (> 2 keV) part shows strong reprocessed features like iron lines $K\alpha$ and $K\beta$ as well as $Ni K\alpha$. Baloković et al. 2014 studied NGC 424 along with other CT sources by using *NuSTAR*, *Swift*/XRT and *XMM-Newton* data. Their analysis further support the presence of a dominant reflection component in the X-ray spectrum, which makes it a good candidate to test our newly developed models. Moreover, Paltani and Ricci 2017 already tested the RXTORUS model on the same source as a benchmark for the model.

We use here both *XMM-Newton* EPIC data and *NuSTAR* FPMA/FPMB to benchmark the RXTOPo and RXAGN1 models. We analyzed the *XMM-Newton* EPIC spectrum of the source using an 8.2 ks observation (ID 0002942301, PI M. Guainazzi) along with a 15.5 ks *NuSTAR* observation (ID 60061007002), which was performed as a part of the campaign to follow up AGN detected by *Swift*/BAT. The observations are the same as those used in Paltani and Ricci (2017). We followed the typical procedures for data reduction and spectral extraction, and details can be found in Paltani and Ricci 2017.

Spectral fitting

For the X-ray spectral fitting, throughout this study we use XSPEC (Arnaud 1996). We set the cosmic abundance to `lpgs` to be consistent with our models. Moreover, all spectra have been rebinned to contain at least 25 counts in each energy bin to apply χ^2 statistics. All errors reported are calculated in the confidence region 90%. For both models we set the Galactic absorption to $N_{\text{Hgal}} = 1.59 \cdot 10^{20} \text{ cm}^{-2}$, as derived by the HI4PI Collaboration et al. 2016.

The first reflection model we applied is RXTOPo. The RXTOPo model consists of a torus that is on the plane of the accretion disk, with a polar hollow cone perpendicular to it, as described in Section 2.2.1. The free parameters of RXTOPo are: the observing angle of the system (θ_o), the photon index Γ of the incident power-law continuum, the equatorial hydrogen column density of the torus ($N_{\text{H}}^{\text{tor}}$), the covering factor of the torus defined as the ratio between the major axis (R) and the minor axis (r) of the torus ($CF^{\text{tor}} = r/R$) and the hydrogen column density of the hollow cone measured along the inner surface of the cone ($N_{\text{H}}^{\text{pol}}$). The softer part of the spectrum shows several spectral features that can be attributed to ionized gas, and

therefore we included an `apec`⁴ model. After several tests, we decided to add a second `apec` component to further improve the fit of the soft X-rays. The free parameter of the two `apec` is the plasma temperature in keV, as well as the normalization. The metal abundance is fixed to the default value (1.0). Finally, a Gaussian emission line is included to reproduce ionized iron (FeXXVI), with width fixed at 10 eV, using the `zgauss` model. The final model in the XSPEC notation is:

$$tbabs \times (rxtopo_{\text{all}} + apec_1 + apec_2 + zgauss) \quad (2.2)$$

The model fits well the data, achieving $\chi^2/dof = 136.05/126$, with a probability of null hypothesis $p_{\text{value}} = 0.255$. The unfolded spectrum and the ratio between the best fit and the data are presented in Fig. 2.7). We find that the photon index is $\Gamma = 1.80^{+0.01}_{-0.01}$, and the observing angle 79.0^{+1}_{-1} . The equatorial hydrogen column density of the torus is $\log(N_{\text{H}}^{\text{tor}}/\text{cm}^{-2}) = 24.48^{+0.03}_{-0.08}$, with a covering factor $CF^{\text{tor}} = 0.66^{+0.02}_{-0.01}$, while the polar cone has $\log(N_{\text{H}}^{\text{pol}}/\text{cm}^{-2}) = 23.19^{+0.04}_{-0.06}$. In order to obtain the line-of-sight column density the simpler approach is to calculate it using the formula:

$$N_{\text{H}}^{\text{los}} = N_{\text{H}}^{\text{tor}} \left(1 - \left(\frac{1}{CF^{\text{tor}}} \right)^2 \cos^2(\theta_{\text{o}}) \right)^{1/2} \quad (2.3)$$

which, for the parameters retrieved from the fit, results in $\log(N_{\text{H}}^{\text{los}}/\text{cm}^{-2}) = 24.46$ or $2.89 \times 10^{24} \text{ cm}^{-2}$. This approach is valid only when the line-of-sight intercepts the dusty torus. In our case, $CF^{\text{tor}} = 0.66$ means that the torus extends up to $\sim 42^\circ$ from the horizon ($\arcsin(CF^{\text{tor}})$), while the observing angle is 79° , which corresponds to just 11° from the horizon. REFLEX also provides an alternative method for calculating $N_{\text{H}}^{\text{los}}$ in any geometry and configuration. We can in fact use the REFLEXINO tool, which is similar to that used to generate Fig. 2.2, 2.4. Details on this approach, and how to build this simulation type are found in Appendix 2.5. Consistent with what expected, the value found with this method is $\log(N_{\text{H}}^{\text{los}}/\text{cm}^{-2}) = 24.46$. The results of the spectral fitting are summarized in Table 2.3.

Next, we apply the RXAGN1 model, which is an extension of RXTOPo that includes the BLR and the accretion disk (Section 2.3.1). The RXAGN1 model has the same free parameters ($\theta_{\text{o}}, \Gamma, N_{\text{H}}^{\text{tor}}, CF^{\text{tor}} = r/R, N_{\text{H}}^{\text{pol}}$) as the RXTOPo. We include two `apec` components, leaving the

⁴<https://heasarc.gsfc.nasa.gov/xanadu/xspec/manual/node134.html>

plasma temperature free to vary with their abundance fixed to the default value; unity. Finally, as done for the RXTOPo model, a Gaussian line is included, with the width set to $\sigma = 10$ eV. The model is:

$$tbabs \times (rxagn1_{\text{all}} + apec_1 + apec_2 + zgauss) \quad (2.4)$$

This model also provides a good fit ($\chi^2/dof = 154.39/126$) with null-hypothesis probability $p_{\text{value}} = 0.044$, and is presented in Fig. 2.8. We find that the photon index is $1.78^{+0.01}_{-0.01}$ and the observing angle $74.9^{+0.4}_{-2.0}$. The column density of the torus is $23.90^{+0.01}_{-0.01}$ for covering factor $\geq 0.90^{+u}_{-0.01}$. The polar cone shows a column density higher than that of the RXTOPo model [$\log(N_{\text{H}}^{\text{tor}}/\text{cm}^{-2}) = 23.80^{+0.01}_{-0.01}$]. In order to find the line-of-sight column density for the current configuration we use the REFLEXINO tool (see Section 2.5). We find that the line-of-sight column density is $N_{\text{H}}^{\text{los}} = 7.59 \times 10^{23} \text{ cm}^{-2}$. The results of this fit are summarized in Table 2.3.

Comparing the two models, we can notice that the values of the two *apec* models and the Gaussian line are consistent within their uncertainties. First, the inclination angle is slightly lower in the case of the RXAGN1 model. For the photon index, the two values lie within the uncertainties. Yet, the parameters that are related to the circumnuclear medium suggest two different configurations. In the case of the RXTOPo model we find a torus that is Compton thick (i.e., $N_{\text{H}}^{\text{tor}} > 10^{24} \text{ cm}^{-2}$) and has an intermediate covering factor ($CF^{\text{tor}} = 0.66^{+0.02}_{-0.01}$). On the other hand, RXAGN1 returns a torus that is thinner, yet close to the 10^{24} limit, with a larger covering factor. Moreover, the polar cone in the RXAGN1 model is denser than the one in the RXTOPo model. Overall, our results show that for NGC 424 we have two scenarios, one that suggests a thick torus but in general low total coverage (torus + cone) and another one that has thinner torus but high total coverage, with extra contribution from the BLR and the accretion disk. The Compton thick scenario of RXTOPo is consistent with the literature (Matt et al. 2000; Baloković et al. 2014; Paltani and Ricci 2017). The RXAGN1 model provides a more complex scenario, where the BLR and the accretion disk contribute to the total absorption, and the torus is thinner but with a larger covering factor. The scope of this analysis is to demonstrate the capabilities of the two new models, and we leave a detailed analysis of NGC 424 to future studies.

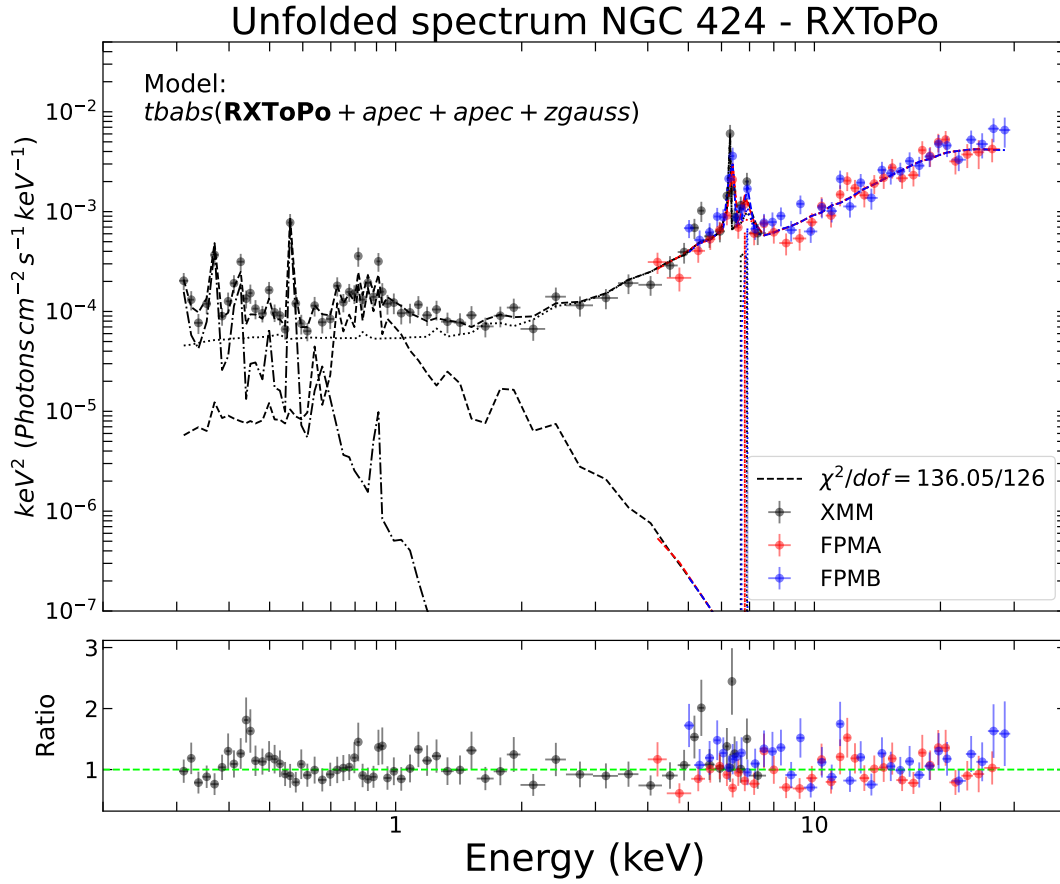


Figure 2.7: The *XMM-Newton* EPIC (black points) and *NuSTAR* (red and blue points) data for NGC 424 along with the best fit model. The individual components are also present. The bottom panel shows the ratio between the data and the model.

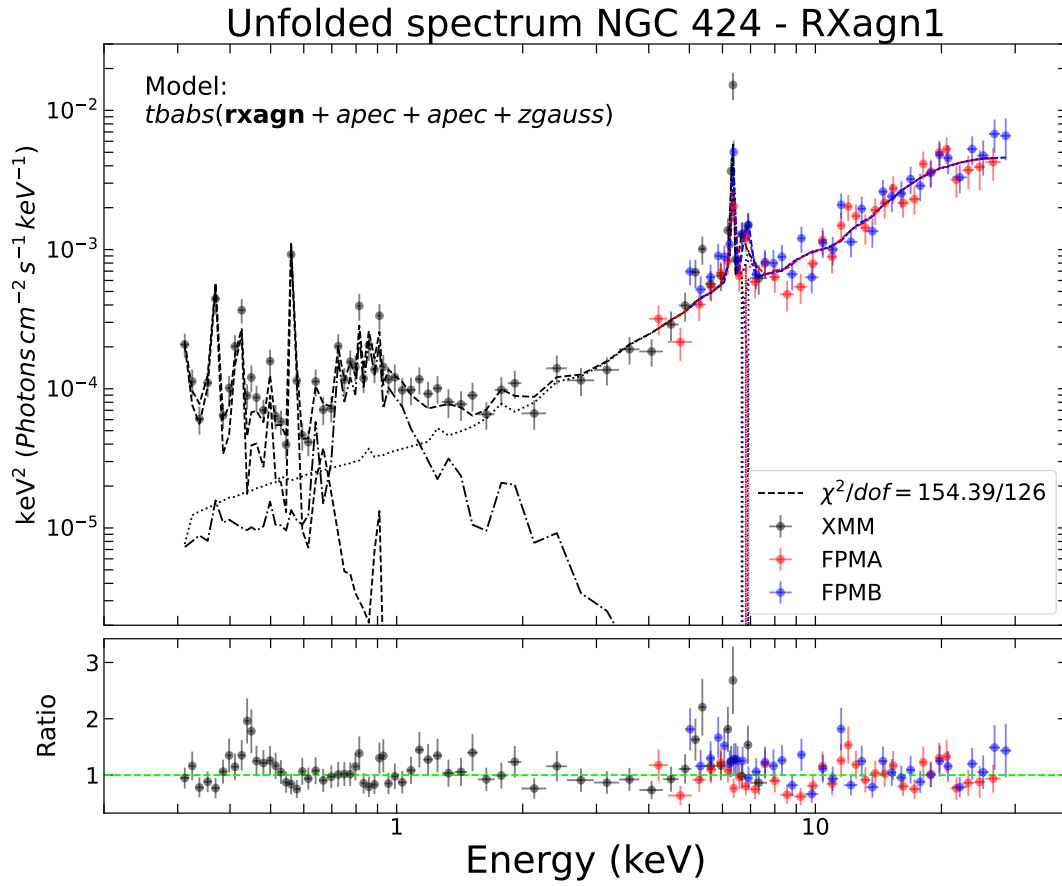


Figure 2.8: The *XMM-Newton* EPIC (black points) and *NuSTAR* (red and blue points) data for NGC 424 along with the best fit model. The individual components are also present. The bottom panel shows the ratio between the data and the model.

Table 2.3: Values obtained from the spectral fitting according to the spectral model $tbabs \times (rxtopo/rxagn + apec + apec + zgauss)$.

	Model	RXToPo	RXagn1
(1)	Angle ($\theta_{\circ}$)	79.00^{+1}_{-1}	$74.9^{+0.4}_{-2.0}$
(2)	Γ	$1.80^{+0.01}_{-0.01}$	$1.78^{+0.01}_{-0.01}$
(3)	$\log(N_{\text{H}}^{\text{tor}}/\text{cm}^{-2})$	$24.48^{+0.03}_{-0.08}$	$23.90^{+0.01}_{-0.01}$
(4)	CF_{tor}	$0.66^{+0.02}_{-0.01}$	$0.90^{+u}_{-0.01}$
(5)	$\log(N_{\text{H}}^{\text{pol}}/\text{cm}^{-2})$	$23.19^{+0.04}_{-0.06}$	$23.80^{+0.01}_{-0.01}$
(6)	$\log(N_{\text{H}}^{\text{los}}/\text{cm}^{-2})$	$24.46^{+0.03}_{-0.08}$	$23.88^{+0.01}_{-0.01}$
(7)	kT (keV) $apec$ #1	$0.10^{+0.01}_{-0.01}$	$0.10^{+0.01}_{-0.01}$
(8)	kT (keV) $apec$ #2	$0.77^{+0.07}_{-0.08}$	$0.76^{+0.06}_{-0.07}$
(9)	Line energy (keV)	$6.91^{+0.09}_{-0.14}$	$6.89^{+0.08}_{-0.11}$
(10)	χ^2/dof	136.05/126	154.39/126

The model parameters are: (1) the observing angle of the system in degrees, (2) the photon index of the cutoff power-law component, (3) the equatorial hydrogen column density of the dusty torus, (4) the covering factor of the torus, (5) the hydrogen column density of the hollow cone, (6) the line-of-sight column density, (7-8) the temperature of the two $apec$ components, (9) the energy of the emission line, (10) ratio between χ^2 and dof . The index u means that the upper limit of the parameter was unconstrained by XSPEC.

2.4 Summary

The analysis of X-ray spectra of heavily obscured AGN often relies on phenomenological models or simplified geometrical models. These models are frequently limited in terms of flexibility and in the range of physical processes they incorporate. In this work, we developed two new models (RXTOPO and RXAGN1) using the ray-tracing platform REFLEX (Paltani and Ricci 2017). The two models cover a wide range of energies, extending from 0.3 to 300 keV and consider a moderate energy resolution (20 eV in the 0.3–10 keV range, and a logarithmic binning of 0.01 above 10 keV). Both models, RXTOPO and RXAGN1, include material that consists of neutral gas and dust featuring all the major interactions between photons and matter (i.e. Compton scattering, Rayleigh scattering, scattering on dust etc; details in Ricci and Paltani 2023). First, the RXTOPO model includes a central X-ray corona, a dusty torus, and a hollow conical polar structure as illustrated in Fig. 2.1 (details in Section 2.2.1). The free parameters of the model are the observing angle (θ_o), the photon index (Γ), the equatorial hydrogen column density of the torus [N_H^{tor} in $\log(N_H^{\text{tor}}/\text{cm}^{-2})$], the covering factor, calculated as the ratio between the inner radius of the toroidal cutout and the distance from the SMBH ($CF^{\text{tor}} = r/R$), and the hydrogen column density of the hollow dusty cone along the inner surface [N_H^{pol} in $\log(N_H^{\text{pol}}/\text{cm}^{-2})$]. All parameters are presented in detail in Table 2.1.

RXAGN1 is an extension of the RXTOPO model (Fig. 2.3). It has the same torus and cone components as RXTOPO plus an accretion disk and a broad line region, both of which have fixed geometry and physical parameters (Section 2.2.2 and Table 2.2). As a result, the free parameters are the same as those of the RXTOPO model.

As described in Section 2.3.1 four different "flavors" are provided based on the type and number of interactions the photons have undergone: all photons (ALL), photons that have undergone at least an interaction with the material (INT), photons that have undergone at least one scattering (SCAT) excluding fluorescent photos, the fluorescence event (FLUO) and the transmitted component, which consists of photons that did not interact with the material (TRNS). This variety of options allows the user to select the one that is most appropriate for the data being analyzed and/or for the physical scenario they wish to adopt.

We tested these new spectral models on NGC 424 (see Section 2.3.2). This obscured AGN

is known to be dominated by reflection and therefore it is a good candidate to benchmark our models. We found that both models can fit well the combined *XMM-Newton* and *NuSTAR* data as illustrated in Fig. 2.7 and 2.8.

Our newly developed models have the potential to constrain the geometry and properties of the circumnuclear material around SMBHs by considering very realistic geometries and physical processes. These models can be used to take advantage of broadband X-ray spectroscopy and, in the near future, high-resolution X-ray observations, such as those that will be carried out by the newly launched *XRISM* observatory and future missions like *Athena*.

Acknowledgments

The authors acknowledge the referees for their useful comments that improved this work. GD acknowledges support from ANID Beca Doctorado Nacional 21211606. The research leading to these results has received funding from the European Union’s Horizon 2020 Programme under the AHEAD2020 project (grant agreement n. 871158). CR acknowledges support from the Fondecyt Regular grant 1230345 and ANID BASAL project FB210003.

2.5 Line-of-sight column density

The best way to calculate the column density that the photons intercept along the line of sight is to use the `REFLEXINO` tool. In this demo, we present how you can use this tool, based on the fit found in Sec. 2.3.2 for the `RXTOPo` model. We need to develop a parameter file (e.g., `my_model.par`) with the proper commands and parameters (for more details, see the manual of `REFLEX`⁵). Here is an example that can be used to calculate the line-of-sight column density for the `RXTOPo` model best fit:

```
VERBOSE 0
NPHOTS 100000
LENGTH Centimeter
EMSPEC REFLEXINO
```

⁵<https://www.astro.unige.ch/reflex/reflex-software>

```

EMGEOM SPHERE 0.0 0.0 5.01534e12 3.0092e12 0.0 0.0 90
OBJECT WORLD 3e30
#OBJECT TORUS EXTERNAL
MATTER lpgs
DUST 1.0
TEMPERATURE 0
H2FRACTION 0.3
METALLICITY 1
DENSITY 2503429.94 #change it accordingly= nh*(2x INNER_RADIUS)
OBJECT TORUS TOR 0.0 0.0 0.0 9.1388e+17 6.0316e+17
#OBJECT HOLLOW CONE
MATTER lpgs
DUST 1.0
TEMPERATURE 0
H2FRACTION 0.3
METALLICITY 1
DENSITY 995.366 #for NH 1e23.19
OBJECT HCONE HCONE 0.0 0.0 0.0 3.1072e+17 1.2343e+20 3.4148e+17 1.3565e+20 2.4015e+
PERCENT ON
HISTOGRAM BINNING 20.0 25.5 0.001 LOG
HISTOGRAM NEW NH NHdeg79.txt
HISTOGRAM DIR_Z < 0.20791169081775945 #78deg
HISTOGRAM DIR_Z > 0.19080899537654492 #79deg

```

The output of this simulation is a text file, in this example `NHdeg79.txt`, that consists of three columns. The first two columns are the left and right bin of the column density and the third column gives the number of photons that have been intercepted in that bin. Normally, the third column should be full of zeros except of the bin that the line-of-sight column density is calculated. In some cases a few bins before and after can be populated with a few photons, but this is not a problem. We consider the bin with the maximum amount of photons to be the correct one. In this case the line-of-sight column density is $N_{\text{H}}^{\text{los}} = 2.89 \times 10^{24} \text{ cm}^{-2}$.

In the case of the RXAGN1 model we need to include the BLR complex and then follow the same procedure.

```
DENSITY 3.2e+09
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 5.6458e+15 5.0119e+15 1.0000e+13
DENSITY 2.5e+09
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 6.3599e+15 5.6458e+15 1.3705e+13
DENSITY 1.9e+09
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 7.1643e+15 6.3599e+15 1.8783e+13
DENSITY 1.5e+09
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 8.0704e+15 7.1643e+15 2.5742e+13
DENSITY 1.1e+09
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 9.0912e+15 8.0705e+15 3.5279e+13
DENSITY 8.9e+08
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 1.0241e+16 9.0913e+15 4.8350e+13
DENSITY 6.9e+08
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 1.1536e+16 1.0241e+16 6.6263e+13
DENSITY 5.3e+08
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 1.2996e+16 1.1536e+16 9.0814e+13
DENSITY 4.1e+08
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 1.4639e+16 1.2996e+16 1.2446e+14
DENSITY 3.2e+08
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 1.6491e+16 1.4639e+16 1.7057e+14
DENSITY 2.5e+08
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 1.8577e+16 1.6491e+16 2.3377e+14
DENSITY 1.9e+08
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 2.0926e+16 1.8577e+16 3.2038e+14
DENSITY 1.5e+08
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 2.3573e+16 2.0926e+16 4.3908e+14
DENSITY 1.2e+08
OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 2.6554e+16 2.3573e+16 6.0176e+14
```

DENSITY 9.0e+07
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 2.9913e+16 2.6555e+16 8.2472e+14
 DENSITY 7.0e+07
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 3.3697e+16 2.9913e+16 1.1303e+15
 DENSITY 5.4e+07
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 3.7959e+16 3.3697e+16 1.5490e+15
 DENSITY 4.2e+07
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 4.2760e+16 3.7959e+16 2.1230e+15
 DENSITY 3.3e+07
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 4.8168e+16 4.2760e+16 2.9095e+15
 DENSITY 2.5e+07
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 5.4260e+16 4.8168e+16 3.9875e+15
 DENSITY 2.0e+07
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 6.1123e+16 5.4261e+16 5.4649e+15
 DENSITY 1.5e+07
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 6.8854e+16 6.1124e+16 7.4896e+15
 DENSITY 1.2e+07
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 7.7563e+16 6.8855e+16 1.0265e+16
 DENSITY 9.2e+06
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 8.7373e+16 7.7564e+16 1.4067e+16
 DENSITY 7.1e+06
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 9.8425e+16 8.7374e+16 1.9280e+16
 DENSITY 5.5e+06
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 1.1087e+17 9.8426e+16 2.6423e+16
 DENSITY 4.3e+06
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 1.2490e+17 1.1087e+17 3.6212e+16
 DENSITY 3.3e+06
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 1.4069e+17 1.2490e+17 4.9629e+16
 DENSITY 2.6e+06
 OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 1.5849e+17 1.4070e+17 6.8016e+16

2.5. Line-of-sight column density

DENSITY 2.0e+06

OBJECT ANNULUS FLAR_DSK 0.0 0.0 0.0 3.1072e+17 1.5849e+17 9.3216e+16

Chapter 3

The Compton Shoulder

This chapter is based on the published paper *The Fe K α Compton shoulder in accreting super-massive black holes* (Dimopoulos et al. 2024). This study is focused on the Compton shoulder (CS) of the Fe K α line. We have explored how the circumnuclear material can affect the shape and flux of the CS, by putting under the microscope various physical properties as well as geometrical configurations.

3.1 Introduction

Fluorescent emission lines (e.g., Fe K α at 6.4 keV) are among the most characteristic features of the reprocessed X-ray radiation observed in AGN. The probability of the emission of a fluorescent line photon is controlled by the fluorescent yield (Y). The Fe K α emission line is possibly the most common feature in the X-ray spectra of AGN due to the relatively high abundance of Fe, and the fact that Y increases rapidly with the atomic number ($Y \propto Z^4$). Fluorescent photons after their emission can interact further with the intercepting medium. Free electrons, bound to neutral or partially ionized electrons are targets of the photons. When Compton scattering occurs between the photons and these "cold" electrons a low-energy tail is formed in energies just below the fluorescence peak, a phenomenon that should not be confused with the up-scattering that takes place in the hot corona where low-energy photons from the disk collide with highly energetic electrons and gain energy through that process. This low-energy tail is a feature known as the Compton shoulder (CS hereafter). Due to the limitations of current X-ray

facilities, this feature has been detected only in a handful of sources (e.g., [Bianchi et al. 2002](#); [Shu et al. 2011](#)). A prominent FeK α CS has been detected in the high-mass X-ray binary (HMXB) GX 301-2 ([Sato et al. 1986](#); [Koh et al. 1997](#); [Nabizadeh et al. 2019](#)). Using *Chandra*-HETG, [Watanabe et al. \(2003\)](#) fit the CS to estimate the column density, electron temperature, and metal abundance of the spherical cloud material that surrounds this X-ray pulsar, which has shown the potential of the CS as a spectral feature that can be useful to constrain the material around accreting objects. [Torrejón et al. \(2010\)](#) studied 31 X-ray binaries (XRBs) using spectra taken by *Chandra*, focusing on the FeK α region, and revealed the presence of a FeK α CS in the HMXB X1908+075. The detection of the CS in AGN is rather rare because of the limited spectral resolution and sensitivity of the current observatories. [Hikitani et al. \(2018\)](#) worked with *Chandra*-HETG data of the *Circinus* galaxy. They were able to resolve the FeK α CS and use it to extract some information about the properties of the obscuring material.

Simulations can be a powerful tool to establish the link between the FeK α CS and the properties of the circumnuclear material of the SMBH. Various works have been performed considering different geometries and physical properties of the circumnuclear environment. [Matt \(2002\)](#) tested the dependence of the CS on the column density and inclination angle, assuming that the reprocessing material is a sphere or a slab. [Murphy and Yaqoob \(2009\)](#) performed Monte Carlo simulations considering that the X-ray source is surrounded by a torus. They also analyzed the FeK α line and the ratio between the fluorescent photons and the scattered ones, which form the CS, finding that for low column densities ($N_{\text{H}} < 10^{23} \text{ cm}^{-2}$) the ratio of the scattered photons over the line photons is very low ($\sim 2\%$). However, as N_{H} increases that fraction also increases, up to $N_{\text{H}} \sim 10^{24} \text{ cm}^{-2}$, and then it drops due to high absorption. [Yaqoob and Murphy \(2010\)](#) performed similar simulations and showed that the shape of the CS is sensitive to changes in the column density of the intercepting material, especially in a high observing angle. For $N_{\text{H}} (> 5 \times 10^{24} \text{ cm}^{-2})$ the CS shows a peak at 6.24 keV, which is the maximum energy shift for 1x scattered photons due to electron recoil for backscattered photons, $\Delta E_{\text{max}} = 2E_{\text{o}}^2 / (m_{\text{e}}c^2 + 2E_{\text{o}})$. They explain that this is related to the inability of photons to penetrate deep into the torus at high optical depths. It was also suggested that flatter spectra, which can provide a higher number of energetic photons, can travel deeper into the medium, so that the spectral index of the incident photon field can also affect the shape of the CS. [Yaqoob](#)

and Murphy (2010) also examined how the velocity broadening of the Fe K α line can blend in with the CS, and illustrated that for velocities $\text{FWHM} > 2000 \text{ km s}^{-1}$, it becomes difficult to distinguish the CS feature, with its only discernible indication being a subtle asymmetry within the blended line profile. Consequently, CCD X-ray detectors lack the capability to identify the Compton shoulder since they feature spectral resolution FWHM of the order of $\sim 7000 \text{ km s}^{-1}$ or more.

Furui et al. (2016) used the MONACO simulation platform (Odaka et al. 2011) and studied the dependence of the CS on different torus parameters. They found a strong relation between the CS intensity and the inclination angle, column density, and metal abundance of the torus. They showed that the ratio between the iron line and its CS depends on the various factors tested, such as the physical properties or the configuration of the torus and whether it is a smooth or clumpy distribution of material. Odaka et al. (2016) investigated how the shape of the CS changes, by using Monte Carlo simulations for spherical and slab geometries of the circumnuclear material. In the case of the spherical medium, they performed simulations testing the column density of the cloud, its metallicity and the spectral slope of the intrinsic continuum. The shape and flux of the CS vary with the physical properties of the sphere (N_{H} , metallicity Z), whereas the photon index (Γ) has no influence on it which can be, however, a result of the moderate column density tested. In the case of the slab reflector they explored the angular dependence of the shape of the CS and showed that the shape of the CS at different angles is characterized by the dominant scattering angle in each case.

The Compton shoulder has not been established yet as an observational feature to probe the properties of the circumnuclear material, due to the lack of high-resolution X-ray observatories. The new generation of X-ray spectrographs, such as the one onboard the recently-launched *XRISM* observatory (XRISM Science Team 2020), will have the necessary spectral resolution and sensitivity to resolve the CS of AGN. In this work, we perform ray-tracing simulations to explore how the physical and geometrical properties of the reprocessing material affect the shape and flux of the Fe K α CS. We use the ray-tracing platform REFLEX (details Section 1.3). Many different properties have been tested such as the composition of metals of the medium (Anders and Grevesse 1989; Wilms et al. 2000; Lodders 2003), the abundance of it (metallicity, Z), the column density (N_{H}) and different dust abundances (Ricci and Paltani

2023). Moreover, the effect of the velocity broadening has been investigated as well as properties of the X-ray source. Besides the physical properties, we use different geometrical objects to form various configurations of the circumnuclear material, by including components such as the accretion disk, the dusty torus, BLR and a polar hollow cone.

In Section 3.2.1 we describe the geometrical objects we use within our simulations. In Section 3.3 we present the results of our simulations organized as following. First, we talk about the physical properties of a toroidal structure and how it affects the CS and then we present the different models of the circumnuclear medium based on the different geometries mentioned above. In Section 3.4 we test the models we have developed on simulated spectra of the next generation of X-ray observatories *XRISM* and *Athena*. Finally, the conclusions of our study are presented in Section 3.5.

3.2 Simulations

3.2.1 Building blocks

The X-ray source

The first component of our simulations is the X-ray source. It is widely accepted that X-ray photons originate in a hot plasma cloud, called corona. The geometry and the position of the corona is still under debate, nevertheless we adopt the lamp-post model which places a spherical corona a few gravitational radii on top of the SMBH (e.g., Fabian et al. 2009; Emmanoulopoulos et al. 2014; Uttley et al. 2014). The location of the corona is fixed at $10r_g$ ($r_g = 2GM_{\text{BH}}/c^2$ is the gravitational radius) and its radius at $6r_g$ (e.g., Chartas et al. 2009; Fabian et al. 2009; De Marco et al. 2013). In order to calculate the distance and the size of the corona, the black hole mass of the Circinus galaxy was used, $\log(M/M_\odot) = 6.23$ (Koss et al. 2017). The shape of the X-ray source can however differ from the typical spherical corona, due to different accretion mechanisms or even the effect of general relativity on the electron population (e.g., Ptak et al. 1998). In Appendix 3.6.1 we test different geometries of the X-ray source to explore their effect on the shape of the CS. We have tested besides the corona described above, a point source as well as an ADAF spherical cloud. None of the tested

geometries changes the shape of the CS. However, it is important to mention that GR effects near the source have not been included in the current work that can affect the overall shape of the spectrum (e.g. [García et al. 2014](#)).

The properties of the input X-ray photons are fixed throughout our study. We generate photons in the energy range 5 – 50 keV to cover the part of the X-ray spectrum known to be dominated by reflection effects, including the FeK α and its Compton shoulder. The energy binning is also fixed at 3 eV, which provides a spectral resolution sufficient to study the CS in detail. The selected photon distribution is a power law with photon index $\Gamma = 1.8$ and energy cut-off $E_C = 200$ keV, in agreement with recent studies of bright nearby AGN (e.g., [Ricci et al. 2017b, 2018](#)). In previous studies, it was tested whether the photon index can affect the shape of the CS (e.g., [Yaqoob and Murphy 2010](#); [Odaka et al. 2011](#)). To explore whether various source properties can affect the FeK α shape and its corresponding CS, in Section 3.6.1 we compare flat and steep spectra for two different toroidal configurations. In our simulations the results of the different spectral indices on the CS is mostly found on the flux of it and not at the shape of it (see Fig. 3.15 which suggests that the CS as spectral feature does not show high potential in constraining the spectral properties of a given source).

To convert the photon counts to observable spectra we fix the AGN luminosity at $L_{2-10} = 3 \times 10^{42} \text{ erg s}^{-1}$, which corresponds to the intrinsic 2 – 10 keV luminosity of the Circinus galaxy ([Arévalo et al. 2014](#)), and the redshift to $z = 0.001$ ([Koribalski et al. 2004](#)). In Table 3.1 the details of the X-ray source are reported.

The accretion disk

In order to explore how X-rays interact with the environment of the SMBH, we need to define different distributions of material around the black hole. The SMBH is surrounded by an accretion disk (AD) that may extend to several hundreds r_g (e.g., [Jha et al. 2022](#)). We created a disk component that starts at $r_{\text{inner}} = 10r_g$ and terminates where the broad line region (BLR) begins at $r_{\text{BLR}} = 0.0037 \text{ pc}$ (see Section 3.2.1). Moreover, the AD is considered to be opaque, and therefore we set the volumetric density at 10^{12} cm^{-3} (e.g., [García et al. 2013](#)). Hydrogen and helium were set to be fully ionized, similarly to the prescriptions used for the PEXRAV model ([Magdziarz and Zdziarski 1995](#)). The metallicity is set to one and the default abundance

Table 3.1: The properties of the X-ray source and the photon distribution of the input radiation field. The source is placed above the SMBH.

Black Hole	
Mass	$10^{6.23} M_{\odot}$
redshift	0.001
X-ray source	
Geometry	Sphere
Distance	$10r_g = 1.62 \times 10^{-6} \text{ pc}$
Radius	$6r_g = 9.75 \times 10^{-7} \text{ pc}$
Γ	1.8
E_c	200 keV
Band	5 - 10 keV
Binning	3 eV

used is `lodd` (Lodders 2003). In our simulation general relativity (GR) effects from the area close to the SMBH are not included and the study of GR on X-ray reflection is outside the scope of this work (see details in García et al. 2014). Nevertheless, the accretion disk and its relative position in the system can work as a giant mirror of cold material which is interesting to explore whether it contributes to the formation of the CS and therefore we decided to implement it. In Section 3.3.2 we show that when any kind of broadening effects are applied to the spectrum the CS becomes less useful as a tool for the study of the circumnuclear medium.

In Fig. 3.1 a cartoon of all the components is presented, including the accretion disk (AD), the properties of which are presented in Table 3.2.

The broad line region

The broad line region (BLR), i.e. the region where broad optical/UV lines are produced, is located after the accretion disk and extends up to the sublimation radius (Suganuma et al. 2006; Davies et al. 2015), where dust is formed. We model it using a flared disk geometry (e.g., Gravity Collaboration et al. 2018, 2020a). To build the flared disk, we used 20 annuli blocks with decreasing inner radius along the vertical axis (see Fig. 3.1). In Appendix 3.6.2 we test different numbers of blocks to recreate the flared disk geometry for the BLR.

The abundance of the BLR is set to `lodd`, the fraction of molecular hydrogen is set to 20% ($H_2 = 0.2$), the volumetric density is fixed for all the annuli at 10^8 cm^{-3} which corresponds to equatorial column density $\sim 10^{25} \text{ cm}^{-2}$ (e.g., Ferland et al. 1992; Goad et al. 2012) and the gas is set to be neutral. The size of the BLR has been calculated considering that its outer radius corresponds to the sublimation radius. First, the sublimation radius was calculated using the following formula (Mor et al. 2009):

$$R_{\text{sub}} = 1.3 L_{46}^{0.5} \times \left(\frac{1500 \text{ K}}{T_{\text{sub}}} \right)^{2.6} \text{ pc} \quad (3.1)$$

where R_{sub} , T_{sub} are the sublimation radius and temperature, respectively, while $L_{46} = L_{\text{bol}}/10^{46} \text{ erg s}^{-1}$. We adopted the 2 – 10 keV luminosity of the Circinus galaxy ($L_{2-10} = 3 \times 10^{42} \text{ erg s}^{-1}$, Arévalo et al. 2014), and converted the X-ray luminosity to bolometric using as bolometric correction $\kappa = 20$ (Vasudevan and Fabian 2009). The inner radius was set to (Kaspi

et al. 2005):

$$\frac{R_{\text{BLR}}}{10 \text{ lt days}} = 0.86 \times \left(\frac{L_{2-10}}{10^{43} \text{ erg s}^{-1}} \right)^{0.544} \text{ pc} \quad (3.2)$$

In Table 3.2 the properties of the BLR are summarized.

The torus

The "torus" is an anisotropic and possibly axisymmetric structure that is found outside the sublimation radius, which was originally proposed in early AGN unification models (e.g., Antonucci 1993; Urry and Padovani 1995). This structure is responsible for obscuring the central region of AGN (e.g., Awaki et al. 1991; Guainazzi et al. 2005, 2016) and reflecting an important amount of radiation (e.g., Matt et al. 1991; Panagiotou and Walter 2019). In Fig. 3.1 we illustrate the toroidal structure and its position in the system. We use the `lodd` abundance and set the molecular hydrogen fraction to $H_2 = 0.3$ and the volumetric density to $\sim 2.2 \times 10^6 \text{ cm}^{-3}$, which corresponds to column density $N_{\text{H}} = 10^{24.5} \text{ cm}^{-2}$. The material is assumed to be neutral. The inner radius is fixed to the sublimation radius, since the torus is expected to be dusty. Hence, the iron depletion factor is set to 70% (DUST=0.7 in REFLEX notation). Moreover, the covering factor is $CF = 0.7$, consistent with the results of recent surveys of nearby AGN (e.g., Ricci et al. 2015, 2017d, 2022). In Table 3.2, we list the properties of the torus.

The cone

Infrared interferometry and single-dish observations of nearby AGN have discovered a warm ($\sim 300 - 400 \text{ K}$) polar dust structure, and a significant fraction of the AGN mid-infrared (MIR) emission could actually be due to this component (Hönig et al. 2014; Asmus et al. 2014; Asmus 2019). In order to implement this polar medium in our simulations, we use a hollow cone that extends up to a few parsecs from the SMBH, a geometry that has been reported for the Circinus galaxy (e.g., Stalevski et al. 2017, 2019). In Fig. 3.1 the polar material is illustrated as a yellow cone. The cone starts at 0.18 pc, which is the distance of the sublimation radius, equal to the one used for the torus, and extends up to 40 pc. Its half opening angle is 40° with outer angle $+10^\circ$, following Stalevski et al. (2017). The volumetric density of the hollow cone is $\sim 62.1 \text{ cm}^{-3}$, which corresponds to $N_{\text{H}} \sim 10^{22} \text{ cm}^{-2}$. The material in the cone is neutral and

has a metallicity $Z = 1$. Moreover, we set the molecular hydrogen $H_2 = 0.4$ (e.g. Wada et al. 2009). Like the torus the polar cone is expected to be dusty and therefore the dust was set to 0.7 too. In Table 3.2 the physical properties of the hollow cone are presented in detail.

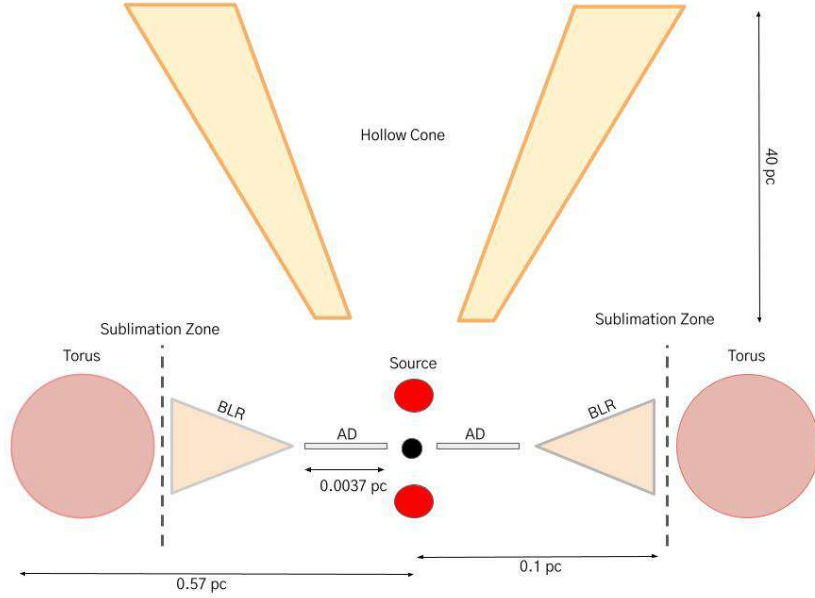


Figure 3.1: Different geometrical components that were considered in our simulations and modeling. Throughout this study various geometrical objects are used. The complete model, composed of all the geometrical objects is the model M6 as described in Section 3.3.3. The objects are not scaled.

3.3 Results

In this section, we present the results of our simulations, which can be divided into two categories. The first set of simulations is focused on exploring different physical parameters of the circumnuclear material and their effect on the CS. For this, we used a simple model to avoid possible degeneracies between the physical conditions and the geometry of the system. The X-ray source is spherical, as introduced in Section 2.2.1 (see, Table 3.1), while the reprocessing medium used is a *torus only* model (see Table 3.2). The properties we tested are: i) metal abundance/composition, ii) metallicity, iii) column density, iv) dust depletion, and v) velocity

Table 3.2: Properties of the different components used in our simulations.

Accretion Disk		Torus	
Geometry	Disk	Geometry	Torus
Inner Radius	$1.625 \times 10^{-6} \text{ pc}$	Inner Radius	0.1 pc
Outer Radius	0.0037 pc	Outer Radius	0.57 pc
Density	10^{12} cm^{-3}	Density	$2.18 \times 10^6 \text{ cm}^{-3}$
State	H, He ionized	Column density	$N_{\text{H}} = 10^{24.5} \text{ cm}^{-2}$
H_2	0	State	neutral
Z	1	Dust	0.7
		H_2	0.3
		Z	1
Broad Line Region		Hollow Cone	
Geometry	Flared Disk	Geometry	Cone
Inner Radius	0.0037 pc	Bottom	0.1 pc
Outer Radius	0.1 pc	Top	40 pc
Density	10^8 cm^{-3}	Angle (width)	40° (10°)
CF	0.4	Density	62.1 cm^{-3}
State	neutral	State	neutral
H_2	0.2	Dust	0.7
Z	1	H_2	0.4
		Z	1

broadening. We decided to refer to metal abundance or composition to the table of metals-elements that correspond to command `abund`¹ in XSPEC. However, metallicity refers to the factor that is multiplied with the densities shown in the aforementioned tables. Moreover, in Appendix 3.6.3 we explored whether the presence of molecular hydrogen can affect the shape of the CS, showing that its effect is negligible. For the second part of our work we fixed the physical properties of the geometrical objects, considering the values reported in Table 3.2. Different geometrical objects were included into our simulations, and their output spectra were compared, in order to explore the diversity in flux and shape of the Fe K α line and its CS.

REFLEX includes the option to select photons based on the type and number of interactions they have undergone from the moment they are generated to the moment they are collected. The scope of this work is to investigate the effect of the circumnuclear material on the Fe K α line and its CS. Hence, we select photons that originate in fluorescence (FLUOR > 0 in REFLEX notation).

The simulated system can be observed in various observing angles via REFLEX. However, throughout our main study we have deliberately limited our analysis in the edge-on scenario (85° – 90° angle width). In previous studies (e.g. [Yaqoob and Murphy 2010](#)) it has been shown that the observing angle can play a role to the observed CS shape and moreover, it is not necessarily a known property in various system, and the different components (e.g. disk and torus) are not always aligned. Nevertheless, in the core analysis of the behavior of the CS we have decided to keep the inclination angle of the system fixed to edge on. Studies of masers suggest a correspondence between high inclination angles and large column densities (i.e. $N_H \geq 10^{23} \text{ cm}^{-2}$), which is also necessary for a strong CS (see Section 3.3.1), (e.g., [Masini et al. 2016](#); [Panessa et al. 2020](#)). Therefore, we decided to keep the inclination angle with respect to the system fixed, and corresponding to a edge-on view, throughout our analysis. However, the reader should be aware of the degeneracies that can be introduced by a varying observing angle. To illustrate it, in Section 3.6.4 we present the Fe K α and CS energy region for different inclination angles. To sum up, unless it is specifically mentioned, the default observing angle bin throughout the main analysis is 85° – 90°.

The effect of the aforementioned properties can be quantified in terms of flux changes on

¹<https://heasarc.gsfc.nasa.gov/xanadu/xspec/manual/node116.html>

the Fe K α emission line ($F_{\text{K}\alpha}$) and its corresponding CS (F_{CS}). To quantify this, we measure the flux of these two components (6.230 up to 6.380 keV and from 6.385 to 6.42 keV for the CS and Fe K α line, respectively), and compare their ratio ($F_{\text{CS}}/F_{\text{FeK}\alpha}$), to study how different physical properties affect the Fe K α line and its CS (see also [Odaka et al. 2016](#); [Furui et al. 2016](#); [Hikitani et al. 2018](#)). All the fluxes are calculated with the continuum subtracted, since we collect only reprocessed photons.

Besides flux changes, the CS can show variations in its shape (e.g., asymmetry). First, to quantify the asymmetry we divide the CS in two branches left and right. The flux of the left branch is integrated from 6.230 up to 6.305 keV and the right one from 6.305 to 6.38 keV and calculate their ratio (asymmetry ratio). Finally, we check how the CS flattens or dents by changing the parameters of the reflecting material. To do that, we consider energy of the Fe K α photons at ~ 6.24 keV as the peak energy of "back-scattering", for the edge-on regime (see also Section 3.6.4, and the lowest flux point in energy range between this "peak" and the emission line (6.28 – 6.38 keV) as "bottom". We calculate the *peak/bottom* ratio to estimate the CS shape. Note that the peak at ~ 6.24 keV is valid for edge-on observations, which is the default configuration. In other observing angles the dominant peak of the CS can significantly deviate from this energy (see Section 3.6.4).

3.3.1 Physical properties

Metal composition

The first property tested is the metal composition of the torus. We ran a series of simulations to examine how different compositions affect the Fe K α emission line and its CS. To do so, we use the option of REFLEX that allows us to select between the most common ones used in the literature. Following XSPEC ([Arnaud 1996](#)) notation² we tested: i) *angr* ([Anders and Grevesse 1989](#)), ii) *wilm* ([Wilms et al. 2000](#)) and iii) *lodd* ([Lodders 2003](#)). The *angr* composition is the one with the highest amount of metals while it has significantly more iron (4.68×10^{-5} , units in comparison to hydrogen) than the other two. The *lodd* and *wilm* compositions have similar Fe abundances, 2.69×10^{-5} and 2.95×10^{-5} respectively, while *lodd* is "richer" in almost

²<https://heasarc.gsfc.nasa.gov/xanadu/xspec/manual/node115.html>

every other element. In general, selecting the metals available in the medium is a way to tune the overall absorption of the incident photons. The total cross-section of the medium changes, and for a given column density this results in different optical depth. As a result, the metal composition is expected to have an influence on the Fe K α and CS.

In Fig. 3.2-top we present the output of the simulations for the three cases described above. For the `wilm` abundances the spectrum has the highest flux, followed by `lodd` and finally by `anгр`. The `wilm` abundance, which has the lowest amount of metals, results in less absorption, and therefore the highest overall flux. This can be better noticed in panel (a) of Fig. 3.2 where the fluxes of both the Fe K α and its CS are presented. Both features show a negative trend, which implies that having more metals increases the overall absorption. The Fe K α line decreases in terms of flux despite the presence of more iron, since the balance between more Fe K α emission and absorption favors absorption. To further test this effect, we have run a series of simulations with the same composition – `lodd` – but variable amount of iron. We found that for Fe abundances from $10^{-2} \times \text{table value}$ up to $10^3 \times \text{table value}$ the overall Fe K α and CS flux drops due to high absorption. In panel (b) of Fig. 3.2 we illustrate the ratio of the two fluxes which shows a slight negative trend but only changes for 0.15. The asymmetry of the three compositions is almost identical which suggests that the different element tables regulate the "amplitude" of the CS but do not affect its shape, which is also supported by what we found for the peak/bottom ratio, which slightly changes as well (see panels (c) and (d) of Fig. 3.2).

In the following we adopt the `lodd` metal abundance as the default option throughout this study (grey line in Fig. 3.2), since it provides sufficient overall flux and produces a significant Compton shoulder feature (see also Table 3.2).

Metallicity (Z)

In the next set of simulations, we investigate how metallicity (Z) affects the Compton shoulder. As discussed in Section 3.3.1, the metals in the torus influence the shape of the CS due to changes in the optical depth of the medium. To explore this, we run a number of simulations covering a range of metallicities from $Z = 0.1 - 2$, considering the `lodd` composition, as described in the previous section. We use the X-ray source and torus described in Section 3.2.1, with the column density and H_2 fraction of the torus fixed to the values reported in Table 3.2,

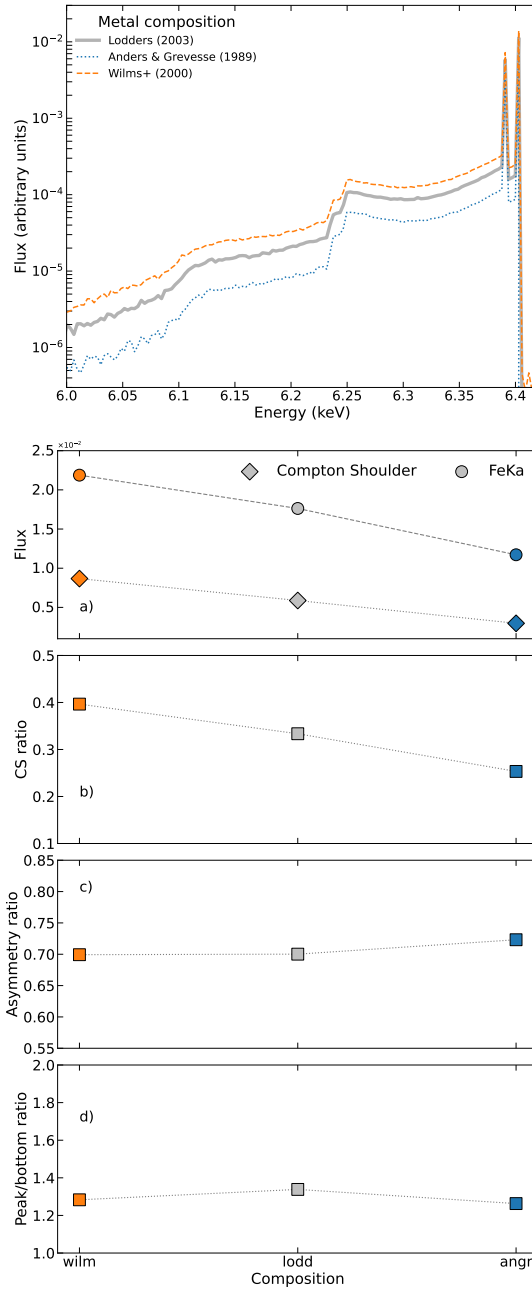


Figure 3.2: *Top*: The Compton shoulder for different metal abundances. The XSPEC notation is used here. In all examples we consider a simple torus, observed edge on, and a spherical corona as the X-ray source. *Bottom*: Top to bottom the four panels show: a) the flux of the CS and Fe K α b) flux ratio CS/Fe K α c) asymmetry ratio and d) peak/bottom ratio.

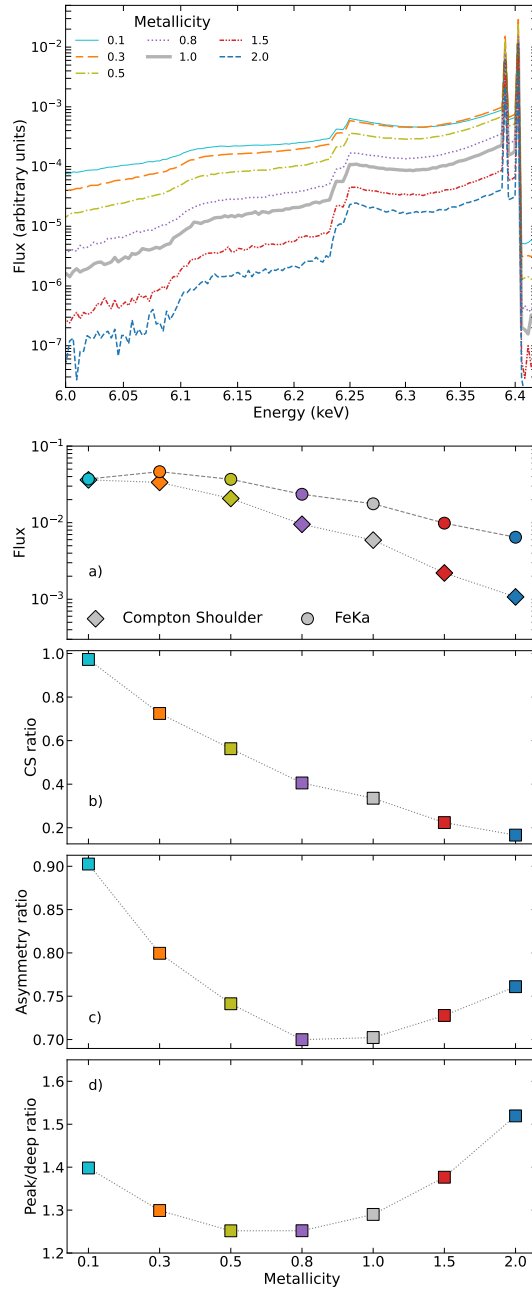


Figure 3.3: *Top*: Spectrum around the Fe K α line for different metallicities. In all examples we use a spherical corona as X-ray source and a simple toroidal reflector. *Bottom*: a) Total flux of the CS and Fe K α b) ratio of the CS flux over the Fe K α line c) asymmetry ratio d) peak/bottom ratio.

$10^{24.5} \text{ cm}^{-2}$ and 0.3 respectively. For these simulations, we assume that hydrogen and helium are neutral.

The top panel of Fig. 3.3 displays spectra around the FeK α line for various metallicities. Increasing the metallicity leads to a decrease in total flux due to greater absorption, consistent with previous studies (e.g., Furui et al. 2016; Odaka et al. 2016). Panels (a) and (b) in Fig. 3.3 show that the flux of the FeK α line and the CS both decline as metallicity increases, and their ratio drops accordingly, indicating that the CS is more affected than the FeK α line. The asymmetry and peak/bottom ratio of the shoulder are shown in panels (c) and (d) of Fig. 3.3. Both indices follow a negative trend up to $Z = 0.8$, without significant in the values of its asymmetry index and an almost stable peak/bottom ratio. However the rapid increase in absorption that occurs for high metallicities ($Z = 1; 1.5; 2$) affects significantly the shape of the CS, resulting in a more asymmetric feature. Our simulations point that both the metal composition and metallicity affect in a similar way the CS.

The effect of metallicity on the CS have been investigated for different geometries by using the MONACO code by Furui et al. (2016) and Odaka et al. (2016). In Furui et al. (2016), a toroidal reflector was used with a central X-ray source, considering both a smooth and a clumpy torus. For the smooth torus, the column density was fixed at $N_{\text{H}} = 10^{24} \text{ cm}^{-2}$ and 10^{25} cm^{-2} , while Z varied from 0.1 to 10. Their results showed that the total flux of the shoulder and the FeK α line drop as Z increases, while the CS gets a more distinctive shape similar to our findings. Moreover, they calculated the ratio between the CS and FeK α flux and found a negative trend with increasing Z similar to the one presented in Fig. 3.3 panel (b). Odaka et al. (2016) performed simulations using a spherical and a slab reflector. For the spherical geometry, N_{H} was fixed at $5 \times 10^{23} \text{ cm}^{-2}$ and Z varied from 0.1 to 10. The results are similar to Furui et al. (2016), showing a decreasing overall flux as the metallicity increases, with a sweet spot at $Z \sim 0.5 - 1.0$, where the CS shows a prominent peak at 6.24 keV. Also, they measured the ratio of the equivalent width of the FeK α over the CS and they found a flat behavior up to $Z \sim 0.5$, followed by a decline for higher metallicities.

Column density

Any means that regulate the optical depths of the intercepting medium affect directly the Fe K α and its CS. This can be achieved either by tuning the concentration of the metals in the medium, as discussed in Section 3.3.1 and Section 3.3.1, or by altering the total amount of material. To test the second factor, we perform a series of simulations using a torus with varying N_{H} . The rest of the settings are similar to the one used in Section 3.3.1. The range of column densities tested is $\log(N_{\text{H}}/\text{cm}^{-2}) = 23.5 - 25.5$.

The spectra of the different simulations are shown in Fig. 3.4-top. It is illustrated that, for column densities $\log(N_{\text{H}}/\text{cm}^{-2}) = 23.5 - 24$, the flux level is significantly higher than for high column densities [$\log(N_{\text{H}}/\text{cm}^{-2}) = 25 - 25.5$], due to the effect of absorption that gradually increases with N_{H} . At high column densities, the shape of the shoulder is characterized by a broad peak around 6.24 keV (back-scattered Fe K α photons). The behavior of the fluxes and flux ratios of the line and the CS is also explored. In Fig. 3.4-bottom we present these ratios for the different column densities. In panel (a) it is shown that the flux of the Fe K α line drops for increasing column densities. The CS flux shows an increase from $\log(N_{\text{H}}/\text{cm}^{-2}) = 23.5$ to 24, while the Fe K α flux slightly drops. As the column density increases both fluxes decline but the Fe K α line shows a steeper decline. This leads to an increase of the relative ratio between the two features as depicted in panel (b). The asymmetry of the CS and the peak/bottom ratio show a similar behavior (see panels (c) and (d) in Fig. 3.4). For low N_{H} there are no significant changes, but the huge drop in total flux for $N_{\text{H}} \geq 10^{25} \text{ cm}^{-2}$ causes a rapid increase in both of these ratios.

Other studies have demonstrated a strong correlation between the CS and column density, using different geometries (e.g., [Matt 2002](#); [Murphy and Yaqoob 2009](#); [Yaqoob and Murphy 2010](#); [Furui et al. 2016](#); [Odaka et al. 2016](#)). The distinct shape of the CS for toroidal geometries with very high column densities ($N_{\text{H}} \geq 10^{25} \text{ cm}^{-2}$) when observed edge on has been first reported in [Yaqoob and Murphy 2010](#). The characteristic back-scattering peak at $\sim 6.24 \text{ keV}$ is a feature that is a combination of the column density (high column density is necessary for sufficient scatterings), the geometry of the system (since for high column densities most of the CS photons are produced in the inner part of the doughnut shaped medium) and the observing

angle which works as proxy of the dominant scattering angle for given N_{H} and geometry. In the next section we explore in detail this phenomenon.

Number of scatterings

The exact location in the obscuring material responsible for the formation of (most of) the Compton shoulder has been debated. [Yaqoob and Murphy 2010](#) tested a toroidal reflector for various column densities and showed that the CS is dominated by FeK α photons that have undergone one scattering, which for large observing angles favors the forward and back-scattering. We ran a series of simulations in which the photons are selected according to the number of scatterings a fluorescent photon undergoes before collected (in REFLEX notation: FLUOR > 0, SCATTER == X; X:1-5). An X-ray source with fixed properties is used (see for details Section 2.2.1, along with a torus featuring metallicity $Z = 1$ and abundance 1_{odd}). Two cases of torus column density are tested. One torus with equatorial column density $\log(N_{\text{H}}/\text{cm}^{-2}) = 24.0$ and another more opaque torus with $\log(N_{\text{H}}/\text{cm}^{-2}) = 25.0$. These two values were selected as examples based on the findings of Section 3.3.1 where the aforementioned values so significant differences (see, Fig. 3.4). Both configurations are observed edge on (see, Section 3.6.4 for details). The spectra formed from the given number of scatterings are presented in the two panels of Fig. 3.5 depicted with different colors. The black solid line with higher flux shows the total flux of the CS and the FeK α for both scenarios. The top panel shows the case of $\log(N_{\text{H}}/\text{cm}^{-2}) = 24.0$. The order of scatterings paves the way to the fluxes and each scattering number gradually contributes less to the CS having less and less flux. Furthermore, no significant changes in the shape of the CS is present. This suggests that photons that have undergone a variety of scatterings come from many parts of the torus which means a plethora of scattering angles and therefore more uniform shape. On the other hand, when the torus becomes even thicker $\log(N_{\text{H}}/\text{cm}^{-2}) = 25.0$ the view changes. First, all the orders of scatterings are concentrated in the same flux levels. Moreover, the shape of the CS between the various scattering numbers changes too. The first scattering (grey-thick line) has a very asymmetric profile depicting the dominance of the back-scattering with a prominent peak at ~ 6.24 keV. The second scattering (blue-dashed line) also has a strong back-scattering peak but in general a smoother CS profile. Higher order scatterings show a flatter profile once again

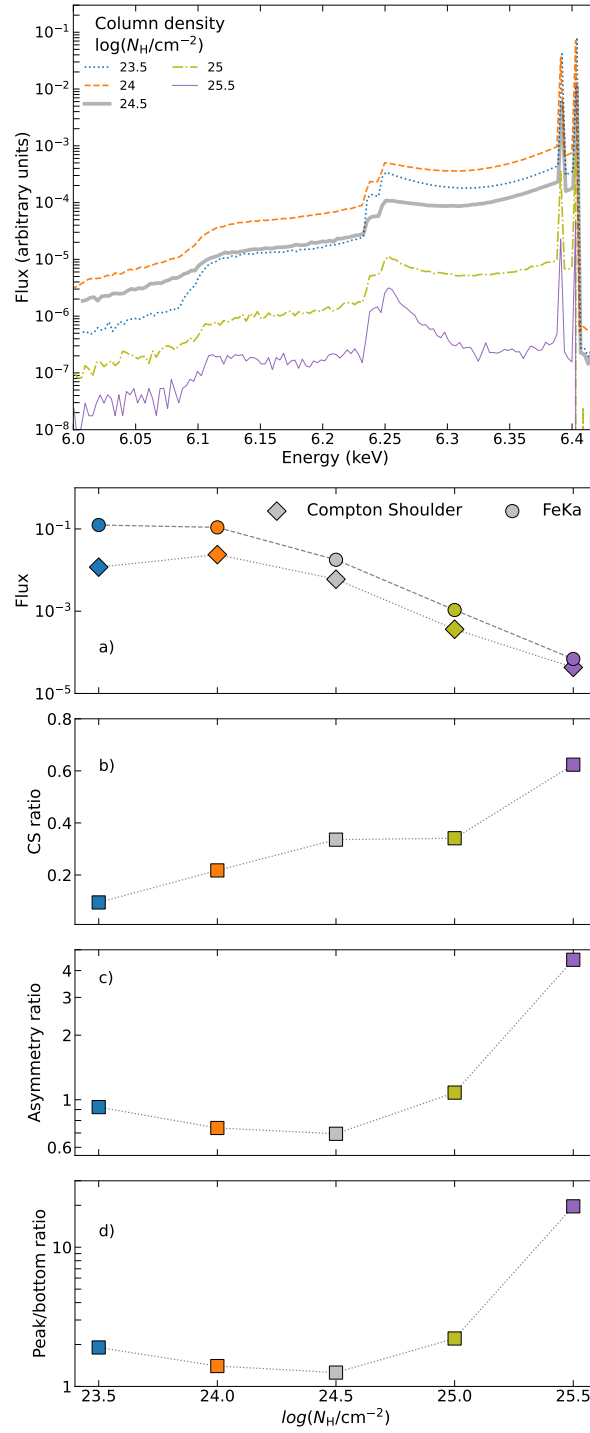


Figure 3.4: *Top*: The Compton shoulder for different torus column densities. *Bottom*: a) The CS and FeK α flux, b) The ratio of the CS flux and the Fe K α line, c) The asymmetry ratio and d) peak/bottom ratio.

reflecting the various scattering angles of the photons that form the CS.

As shown in the bottom panel of Fig. 3.5, for high column density ($N_H = 10^{25.0} \text{ cm}^{-2}$) the shape of the spectrum changes depending on the number of scatterings. We explore the region in the torus where they last scattered before being collected by the detector. To do that we used the option of REFLEX to generate images. We used the exact same configuration as described in Table 3.2, with the source properties fixed to those reported in Table 3.1. The equatorial column density was set to be $\log(N_H/\text{cm}^{-2}) = 25.0$. To see how the CS is formed, we created images by collecting the photons that fall in the 6.20 – 6.42 keV energy range (Fig. 3.6). We show the toroidal reflector from three different observing angles, so that the inner regions can be easily observed at low angles ($\sim 10^\circ$), while being "obscured" at higher inclination angles ($\sim 80^\circ$). Each panel shows the images that we reconstructed by collecting photons based on the number of scattering from one to four. In the previous paragraph (see, Fig 3.5) the fifth scattering is included as well but it does not show any significant difference with the fourth one and therefore for clarity we omitted it in this case. The high asymmetry of the first scattering arises primarily from forward and back scattering due to the energy loss profile associated to Compton scattering. These scatterings take place in the inner surface of the doughnut shape torus (see also Yaqoob and Murphy 2010; Furui et al. 2016). This is illustrated as the brighter central regions observed in the first scattering, especially when viewed from above (10 degrees), where the inner surface is directly exposed. While the second scattering also exhibits some asymmetry with a brighter center, higher-order scatterings show a more uniform light distributions, as shown by the consistent blue color across the images.

Dust

The presence of dust in the torus is expected since it extends beyond the sublimation radius, as discussed in Section 2.2.1. In the most recent version of REFLEX (Ricci and Paltani 2023), the user can adjust the amount of dust particles by changing the *dust depletion* parameter (DUST), which controls the fraction of metals that are bound in dust grains. To investigate whether dust affects the shape of the CS, we followed the same approach as in Section 3.3.1 (see Table 3.2) and varied the dust depletion factor to DUST 0, 0.7, and 1.0, which correspond to fractions of iron bound in dust grains of 0%, 70%, and 100%, respectively.

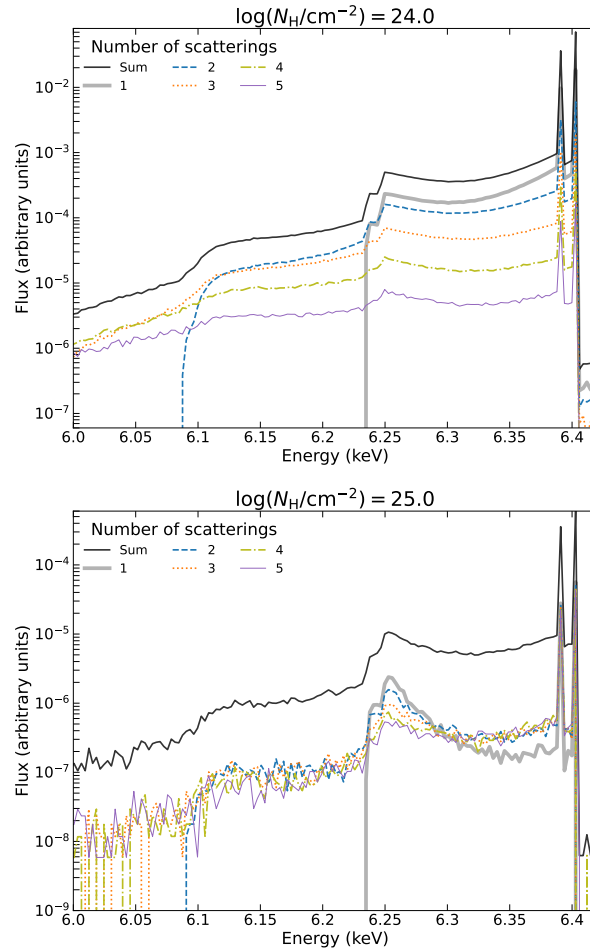


Figure 3.5: The Fe K α and CS spectrum formed by fluorescent photons that have undergone a specific number of scatterings (1 to 5). The black line ("sum") is the total spectrum including all the scatterings. The model consists of a spherical corona and a torus, with fixed physical properties $Z = 1$, ι_{odd} in two different column density scenarios. *Top*: A torus with column density $N_{\text{H}} = 10^{24.0} \text{ cm}^{-2}$. *Bottom*: A torus with column density $N_{\text{H}} = 10^{25.0} \text{ cm}^{-2}$.



Figure 3.6: Images generated with REFLEX for a torus with $\log(N_{\text{H}}/\text{cm}^{-2}) = 25.0$. Each image is created by collecting photons based on the number of scatterings it has undergone before collected. From left to right are presented three different observing angles. The high asymmetry on the Compton shoulder that was found for high N_{H} and low number of scatterings it is illustrated in the yellow core of each doughnut.

In Fig. 3.7-top the spectrum at the Fe K α line and CS region is presented. It is clear from the comparison between spectra with different depletion values, that the presence of dust does not affect neither the Fe K α emission line nor its CS. Ricci and Paltani (2023) tested the effect of dust on fluorescent lines that originate from elements that can be found in dust grains, such as oxygen, carbon, magnesium, silicon and iron. No significant difference in the properties of fluorescent lines was found in their work.

3.3.2 Velocity broadening

So far we have investigated configurations of tori that can vary in terms of their physical conditions. These physical properties can affect the shape of the Fe K α and its CS (i.e. column density) or have zero impact like the presence of dust grains.

However, in the aforementioned simulations we did not take into account potential velocity broadening on the emission line due to various effects such as Keplerian motions of the circumnuclear material.

In fact, any kind of broadening on the Fe K α complex can affect the resulting spectrum. Broad Fe K α lines have been observed in several AGN in which the broadening can be at-

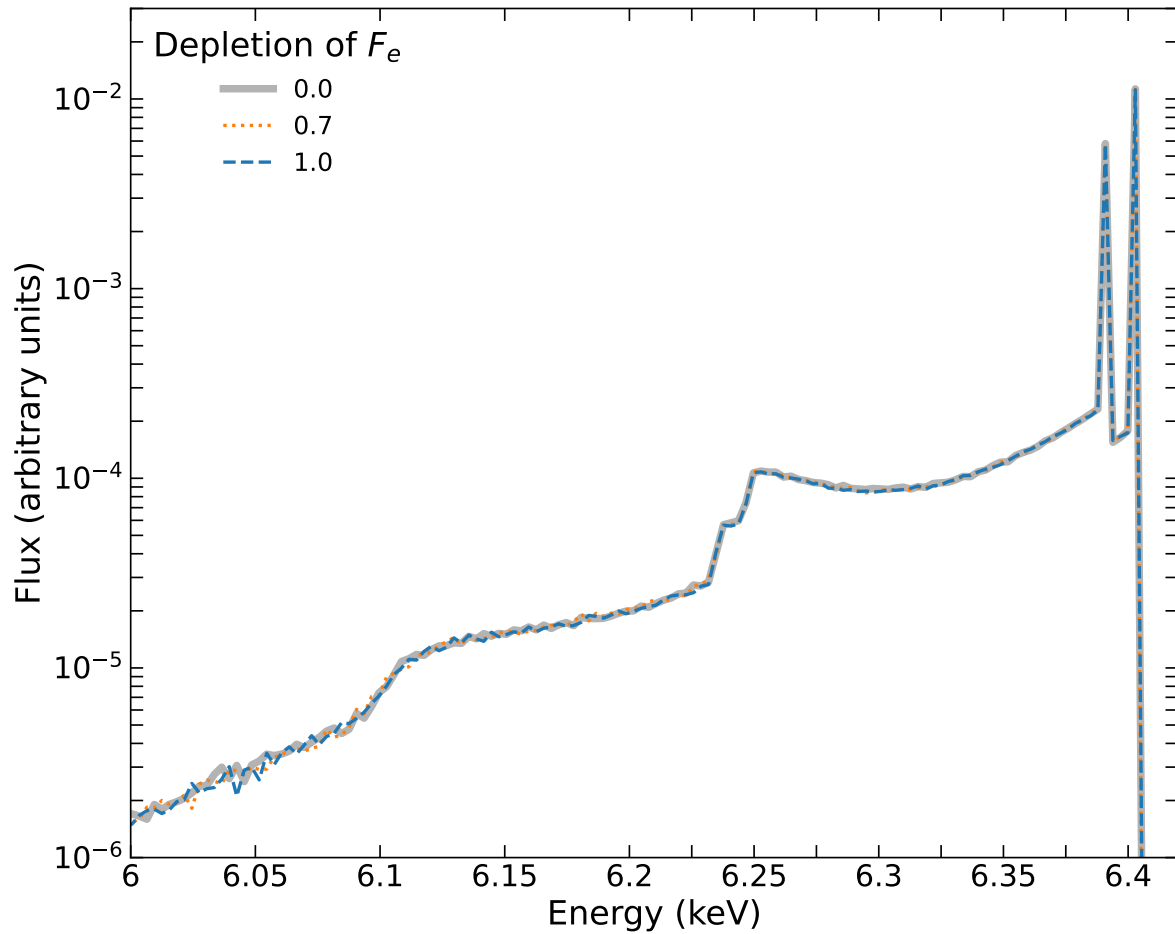


Figure 3.7: *Top*: The Compton shoulder for different values of dust depletion. In all examples we use a spherical corona as X-ray input source along with a torus, observed edge on, with varying dust fractions.

tributed to the revolution of chunks of gas at different velocities based on the distance from the central SMBH (e.g., [Shu et al. 2010, 2011](#)); an effect that should not be confused with the relativistic broadening that can also be observed which is a result of the general relativity and is often accompanied by distorted soft X-ray spectral features (e.g., [Brenneman and Reynolds 2009](#)). In this section the goal is not to breakdown the different velocity components of the Fe K α or to use the CS to constrain such velocities. On the contrary we introduce an ad-hoc gaussian broadening to the spectra to emphasize to the fact that the Compton shoulder as a tool to constrain the physical properties of the circumnuclear medium, presents many limitations when the Fe K α complex is affected by any kind of broadening effects. The version of REFLEX that is used throughout this analysis does not include any kind of motions to the material. Yet, another version is under development that implements such physical mechanics. Nevertheless, available tools in X-rays, such as SKIRT ([Vander Meulen et al. 2023](#)), can be used for a detailed analysis of velocity effects in various media and configurations. Here, we adopt the same configuration with the previous paragraphs to test the effect of the velocity broadening on the Fe K α and its CS. A simple torus with its physical properties fixed to the values of Table 3.2 is used. In Section 3.3.1 we have shown that the column density of the torus can affect the shape of the CS and it can lead to less or more distinctive shapes. A clear difference is noticed between a torus with $\log(N_{\text{H}}/\text{cm}^{-2}) > 24.5$ and one with column density less than that, with the first showing higher asymmetry whereas the latter a flatter CS as seen in Fig 3.4. Hence we decided to test the velocity broadening effect in two cases. One for $N_{\text{H}} = 10^{24.5} \text{ cm}^{-2}$ and one for $10^{25.5} \text{ cm}^{-2}$. We apply in the output spectrum of REFLEX the gaussian function `gsmooth`³ from XSPEC to take into account the velocity broadening. The width of the broadening is:

$$\sigma_{\text{E}} = \sigma_{\text{L}} \left(\frac{E}{6 \text{ keV}} \right)^{\alpha}, \quad (3.3)$$

where

$$\sigma_{\text{L}} = 0.85 \left(\frac{V_{\text{FWHM}}}{100 \text{ km/s}} \right) \text{ eV}. \quad (3.4)$$

Using *Chandra*/HETG data [Shu et al. \(2010, 2011\)](#) studied extensively the Fe K α emission line in several nearby type I and type II AGN providing tables with the FWHM of the line for each source. The velocity broadening reported in these works spans from a few thousands to tens

³<https://heasarc.gsfc.nasa.gov/xanadu/xspec/manual/node288.html>

of thousands km s^{-1} . We have adopted three different values: 1000, 2000 and 5000 km s^{-1} which correspond to $\sigma_L = 8.5, 17, 42.5 \text{ eV}$ respectively, for $\alpha = 1$. The different velocities suggest that fluorescence originates in different regions, with higher velocities to be related to the broad line region and the lower ones to material that is even further like the dusty torus. In Fig. 3.8 the results obtained for the different velocities are presented along with the zero velocity spectrum (grey line). It is clear that for 1000 and 2000 km s^{-1} the $\text{Fe K}\alpha$ line and the CS are still clearly distinguishable. Although the doublet of the line is diluted and the back-scattering peak of the CS is stretched it still maintains the "shoulder" shape. In the high-velocity case (i.e. 5000 km s^{-1}) the complex of the $\text{Fe K}\alpha$ line and the CS are entirely smoothed. Nevertheless, if we compare the shape of the $\text{Fe K}\alpha$ and its CS between the two column densities tested, it is clear that the overall shape is significantly difference. For $N_H 24.5$ the slope is smoother from lower energies to the $\text{Fe K}\alpha$ energy whereas for $N_H 25.5$ a bumpy shape is produced. The distinct shape between the two implies that even though the complex ($\text{Fe K}\alpha + \text{CS}$) is blended, the overall information for the column density of the material is maintained. Overall, it is clear that rapidly moving material can limit the potential of the CS as a diagnostic tool for the properties of the circumnuclear material.

3.3.3 Geometry of the circumnuclear material

In the previous paragraphs, we illustrated the effect of the physical properties of the obscuring medium on the shape and flux of the $\text{Fe K}\alpha$ line and its Compton shoulder. Previous studies have focused on the physical properties of the circumnuclear material using simple geometries and considering only one geometrical object in each simulation. In this section, we introduce different geometries of the medium surrounding the SMBH, using the option of REFLEX that allows the user to add different geometrical objects (see Section 1.3). In Fig. 3.1 all the components that are used to build complex models are presented.

We run simulations with increasing complexity, starting from a simple slab geometry and then moving to more complex AGN models, based on the geometrical objects introduced in Section 3.2.1. We fixed the physical properties of the different components to the values reported in Table 3.2. We consider a spherical corona as X-ray input source and collect the

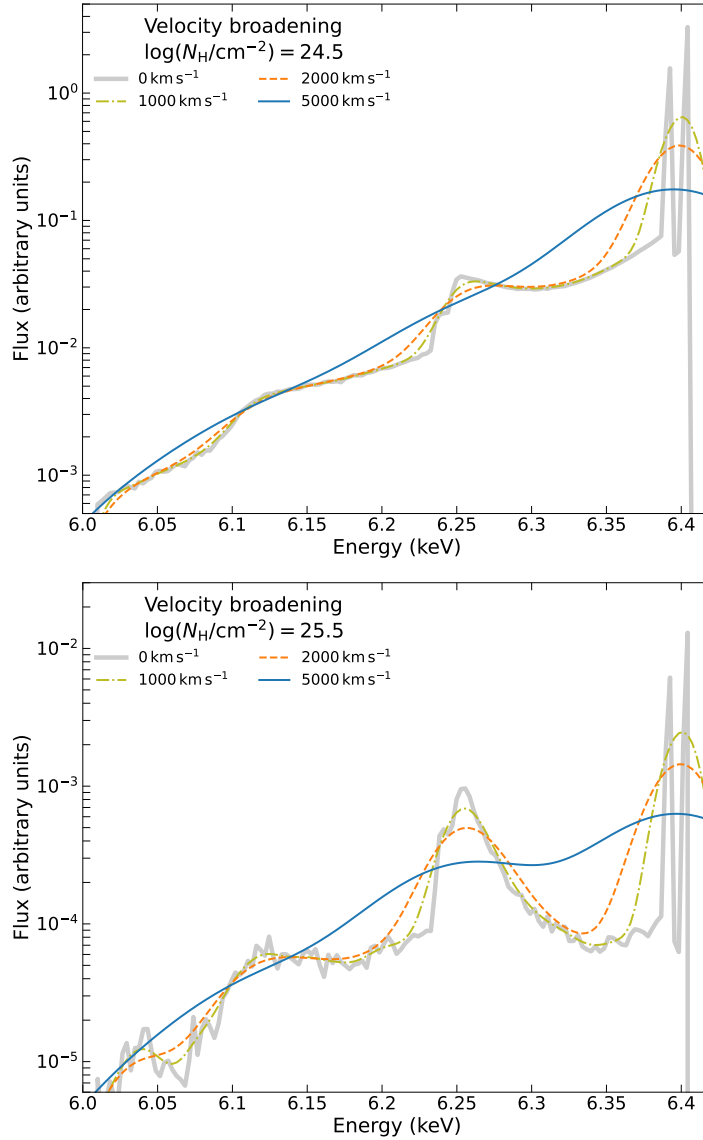


Figure 3.8: The FeK α energy region along with its CS formed by a simple toroidal reflector. *Top*: The panel shows the spectrum for a torus with $N_{\text{H}} = 10^{24.5} \text{ cm}^{-2}$. The different colors represent different gaussian broadening that has been applied to the raw spectral output of the simulation. *Bottom*: Same exercise for a torus with higher column density.

photons that originate from fluorescence. We begin by testing a simple slab geometry (M1). To model this we use the accretion disk component with fixed physical properties to the ones presented in Table 3.2. Next, we test a corona inside a homogeneous spherical medium (M2), to see how the presence of isotropic material can change the shape of the CS. For the spherical medium we use a sphere with center at the SMBH that extends up to the sublimation zone. This sphere has neutral gas with no dust and column density $N_{\text{H}} = 10^{24.5} \text{ cm}^{-2}$. We include in our analysis the torus component (M3) that we used in the previous sections too. We then consider a more complex model which includes an accretion disk along with the torus (M4). Next, we build a model (M5) that includes an accretion disk, torus and the broad line region (BLR). The last model (M6) combines the accretion disk, the BLR, the torus and a hollow cone. For the aforementioned geometries we test two different scenarios regarding the observing angle, one for 45° and one for 90° .

The spectra focused on the Fe K α line region are illustrated in Fig. 3.9. The top panels show the spectra, whereas at the bottom panels the fluxes and ratios can be found. First, for the case of the disk geometry (M1) we can see that the flux level for both observing angles is similar. The shape of the CS, however, shows a different peak based on the scattering angle. Different observing angles favor the collection of photons that have been scattered for different angles as shown in details in [Yaqoob and Murphy 2010](#). In Appendix 3.6.4, we further test the effect of the observing angle on the CS in the case of slab geometry (see Fig. 3.18). For the case of the spherical surrounding material (M2) the flux of the CS is consistent for both angles since it is a fully symmetric configuration. As seen in Fig. 3.9 panel (c) the spherical CS is smoother or less asymmetric another effect the isotropic nature of the spherical geometry. Models M3, M4, M5 and M6 include the torus, which is the main medium that reprocess the photons in the edge-on regime and introduces asymmetry to the system. The CS is almost indistinguishable in the case of 45° angle, something that can be confirmed by the bottom panels (a, b, c, d) of the left panel in Fig. 3.9. When the system is observed edge on (90°), the presence of the BLR (M5, M6) adds as an extra layer of material between the observer and the source and hence, the flux of the CS and the Fe K α drops. The hollow cone that is included in M6 does not affect the CS significantly as a result of the low column density of the polar medium.

Overall, it is clear that the slab reflector is a special case of reflecting material something

that is also seen in Fig. 3.18. Moreover, the spherical geometry can also be distinguished due to its symmetrical shape with no favorable scattering angle. Last, all the models that introduce axisymmetry (simple torus M3, torus+disk M4, torus+disk+BLR M5 and and torus-disk-BLR-hollow cone M6) have similar results and it is difficult to distinguish between geometries. On the contrary the main factor that affects the shape of the CS is the total line-of-sight column density.

3.4 Simulated XRISM and Athena spectra

The Compton shoulder could be a useful tool to constrain some of the properties of the circumnuclear material. Current X-ray facilities have limited resolution in the 6 – 7 keV band and so far the CS has been detected only in a handful of nearby objects (e.g., Sato et al. 1986; Watanabe et al. 2003; Torrejón et al. 2010; Hikitani et al. 2018). Future instruments like XRISM/Resolve (XRISM Science Team 2020) and Athena/X-IFU (Barret et al. 2016) will have the necessary spectral resolution (5 – 7 eV and 3 eV for Resolve and X-IFU, respectively) and sensitivity to make the Fe K α CS a useful observable spectral feature.

We used REFLEX to create a realistic model of the Circinus galaxy, since it is one of the X-ray brightest nearby heavily obscured AGN, and it is known to show a Fe K α CS feature (Bianchi et al. 2002; Hikitani et al. 2018). Since the CS has not been observed in other AGN and as a result it cannot be considered a diagnostic tool yet, it is reasonable to start from a source with an observed CS. Nevertheless, this does not guarantee that in other sources the CS can be effective. We ran a simulation using the model M6, which consists of an accretion disk, BLR, dusty torus and polar medium (see Section 3.3.3), a schematic of which can be found in Fig. 3.1. The physical properties of the different components of the model are fixed to the values reported in Table 3.2. The column density of the torus is set to $N_{\text{H}} = 10^{24.5} \text{ cm}^{-2}$ and the metallicity $Z = 1$, values that are close to the ones reported in recent studies of the Circinus (e.g., Andonie et al. 2022). The flux level used is the observed 2 – 10 keV flux of Circinus reported by Ricci et al. 2017b and the observing angle is fixed to 78° (Arévalo et al. 2014; Andonie et al. 2022). Velocity broadening around the Fe K α line has been reported in Circinus, with average value estimated to be $\text{FWHM} = 1346 \text{ km s}^{-1}$ (Andonie et al. 2022). To

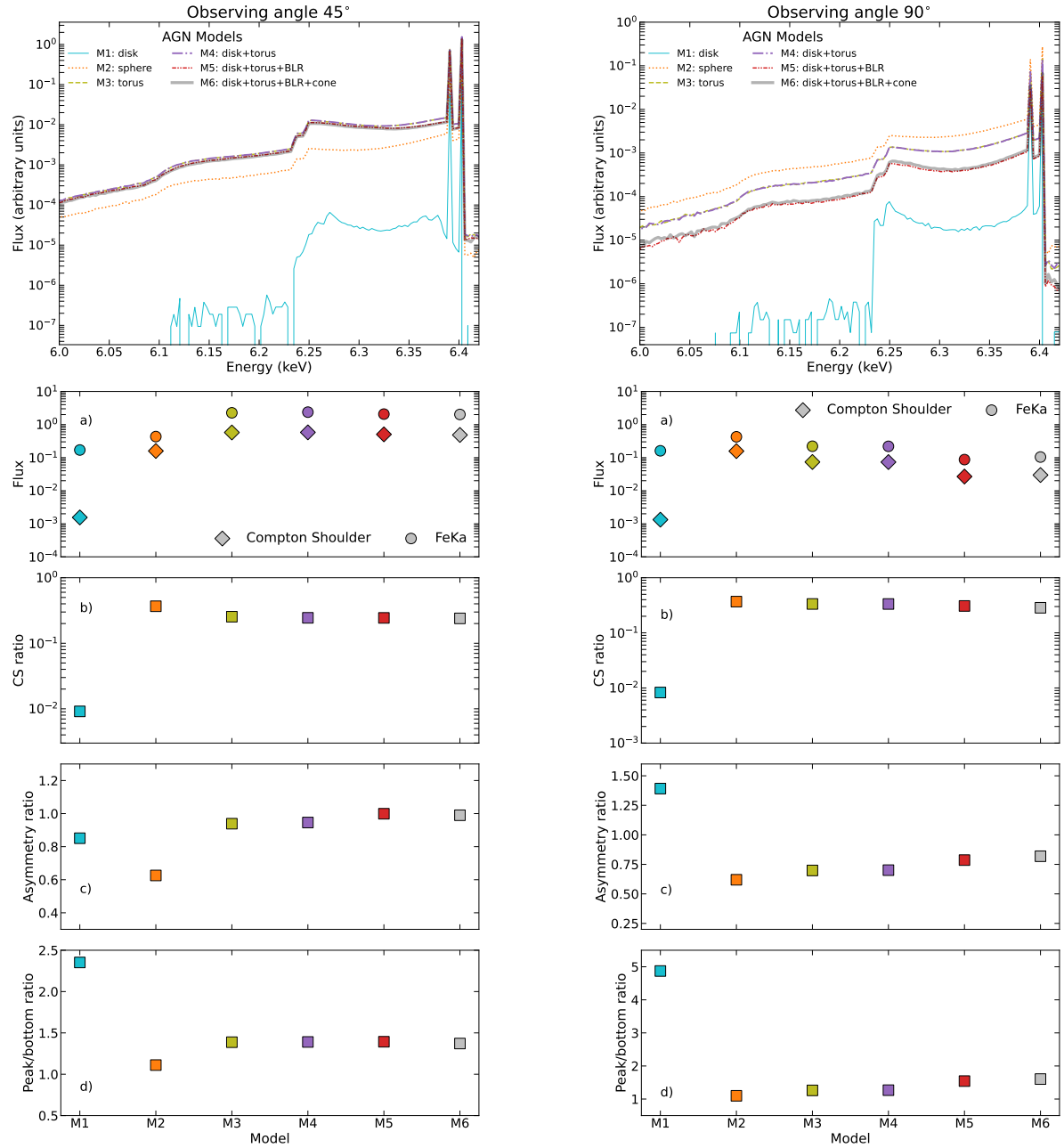


Figure 3.9: *Top panels:* The CS and the FeK α for different geometries observed in 45° (left panel) and 90° (right panel) inclination angle. The models consists of the components presented in Fig. 3.1, with their physical parameters fixed to the values from Table 3.2. The models: M1: *Disk*, M2: *Sphere*, M3: *Torus*, M4: *Disk + Torus*, M5: *Disk + Torus + BLR*, M6: *Disk + Torus + BLR + Hollow Cone*. *Bottom panels:* a) The CS and FeK α flux, b) The ratio of the CS flux and the FeK α line, c) The asymmetry ratio and d) peak/bottom ratio.

include the effect of velocity fields, we used `gsmooth` from XSPEC similarly to Section 3.3.2 setting $\sigma_L = 11.44 \text{ eV}$ and $\alpha = 1$, which corresponds to the FWHM above.

To generate the simulated spectra the X-ray analysis package XSPEC was used along with the response files of the Resolve⁴ and X-IFU⁵ instruments, including their respective background files. The exposure time for the simulated spectra was set to 200 ks, which provides sufficient signal-to-noise to reveal the CS feature. For the analysis and the fitting of the simulated data we used XSPEC too. The spectra are rebinned so there is at least one data point in each energy bin (`group min 1`). Cash statistics (Cash 1979) are applied and the errors when constrained successfully were calculated in 90% confidence level throughout our analysis. After simulating spectra for both instruments, we conducted two tests to evaluate the effectiveness of the CS, focusing on the energy range 6.0 – 8.0 keV, which is expected to be dominated by reprocessed radiation for the Circinus galaxy. First, we test whether the input parameters of the simulated spectrum can be retrieved, such as Γ , σ_L (FWHM), N_H and Z . Then, we applied three different geometrical models from Section 3.3.3 - torus, sphere, M6 model - to investigate whether the FeK α and its CS as a spectral feature can differentiate between the given geometries.

3.4.1 Testing the physical properties of the torus

We develop a grid spectral model considering the M6 geometry, which was introduced in Section 3.3.3 and includes all the main component of AGN (disk, BLR, torus, polar cone). Our grid model has been implemented having three free parameters, the spectral index (Γ), the column density (N_H) and metallicity (Z) of the torus. The properties of all the other components are set to the values presented in Table 3.1 and 3.2. The primary continuum spectral index was set with three different values, 1.5, 1.8, 2.4. Similarly, metallicity was set to values: $Z = 0.5, 1.0, 1.5$. The N_H spans between $\log(N_H/\text{cm}^{-2}) = 24$ and 25 with steps of $\Delta \log(N_H/\text{cm}^{-2}) = 0.1$.

We performed simulation generating photons from 5 to 50 keV, collecting the 6 – 8 keV energy range with 3 eV binning, so as to achieve good signal to noise in reasonable computational times. Having developed the necessary grid output we compiled them in one table

⁴<https://heasarc.gsfc.nasa.gov/FTP/xrism/prelaunch/simulation/sim3/>

⁵<http://x-ifu.irap.omp.eu/resources/for-the-community>

model and imported in XSPEC. We employed this grid model to analyze the simulated spectra from *XRISM* and *Athena* to determine whether the input properties can be retrieved. We fit the data, in the 6 – 8 keV band, using `gsmooth(M6model)` so as to take into account the velocity broadening. We fit the Circinus *XRISM*/Resolve simulated spectrum and we get $\text{FWHM} = 1338_{-26}^{+27}$ km/s, $\Gamma = 1.78_{-0.14}^{+0.16}$, $\log(N_{\text{H}}/\text{cm}^{-2}) = 24.49_{-0.05}^{+0.05}$ and metallicity $Z = 0.995_{-0.018}^{+0.080}$. The model is able to well fit the data ($C\text{-stat}/dof = 0.96$). In the left panel of Fig. 3.10 we illustrate the simulated spectrum in the 6-8 keV band along with the best fit. The bottom panel shows the residuals. The right panel of Fig. 3.10 is focused on the FeK α line energy region. The model provides a good fit and succeeds in constraining the spectral index accurately. For the remaining three properties FWHM, N_{H} and Z it returns values marginally lower than the input ones, even if we consider the errors which are small. This can be attributed to systematic errors that have not been taken into account.

Next, we apply the same model on the *Athena*/X-IFU spectrum (see Fig. 3.11). In this case the fit is also good ($C\text{-stat}/dof = 0.97$) similar to the *XRISM* example. The constrained values are: $\text{FWHM} = 1337_{-11}^{+10}$ km/s, $\Gamma = 1.75_{-0.07}^{+0.04}$. The column density is $\log(N_{\text{H}}/\text{cm}^{-2}) = 24.50_{-0.03}^{+0.05}$ whereas the metallicity is found $Z = 0.991_{-0.008}^{+0.024}$.

Overall, we see that, with the advent of new X-ray facilities, modelling of the FeK α region can contribute to the understanding of the physical conditions of the circumnuclear material. In our example the simulated spectra and the model used to fit that are the same and therefore the result cannot be considered as robust evidence for the derived values of the properties. However we consider it as a useful exercise to illustrate how the 6 – 8 keV band will look with microcalorimeters, as well as explore some profound degeneracies between the properties.

3.4.2 Testing different geometries

It has been illustrated that the physical properties can be retrieved by fitting the CS even with some deviations from the input values. Despite that, we are interested in testing whether the CS can be used as a tool to distinguish between different geometries. In Section 3.3.3 several configurations have been tested. We adopt the following three geometrical models and run simulations using REFLEX. The models are: i) sphere (M2), ii) torus (M3), and iii) M6 (disk,

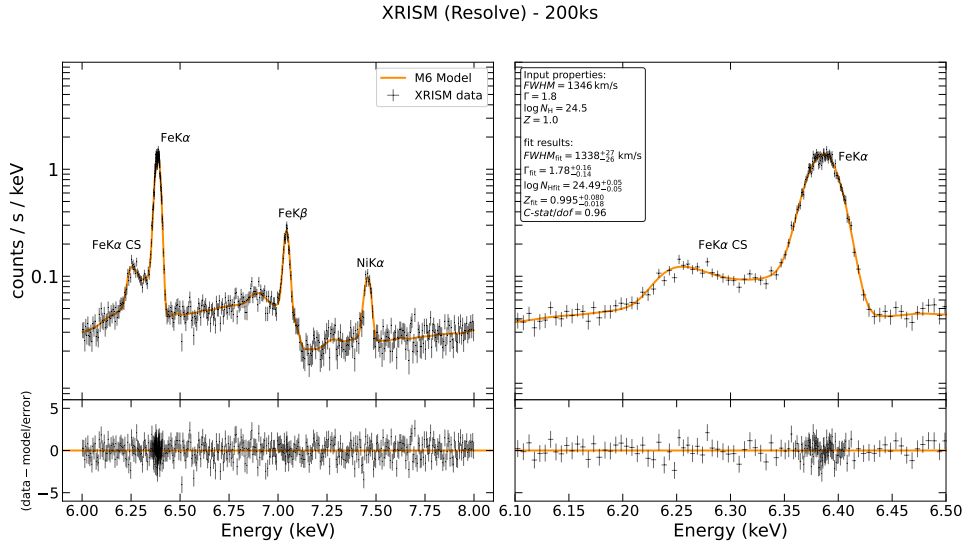


Figure 3.10: The simulated spectra of Circinus around the Fe K α line region. The spectra are fitted with a grid model developed using the M6 geometry (see Section 3.3.3) Free parameters are the N_{H} and Z . In the left panel the XRISM/Resolve data along with the data/model ratio are presented. The orange line is the best fit with the retrieved values summarised in the box.

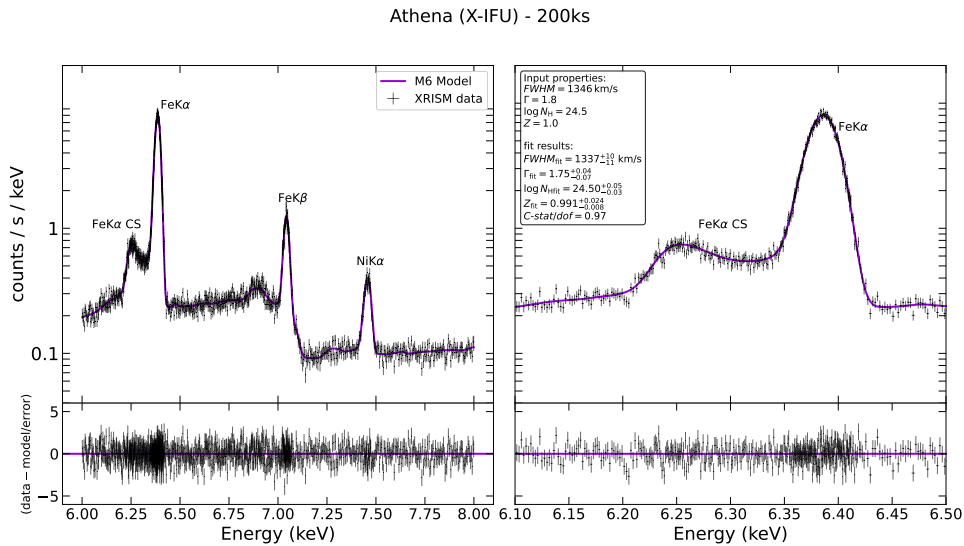


Figure 3.11: The simulated spectra of Circinus around the Fe K α line region. The M6 geometry (see Section 3.3.3) has been used to generate a grid model with having free parameters the N_{H} and Z . In the left panel the Athena/X-IFU data along with the data/model ratio are presented. The orange line is the best fit with the retrieved values summarised in the box.

BLR, torus, polar cone) from Section 3.3.3, as they show variations in the shape of the CS (see Fig. 3.9). The three grid models have the same free parameters; N_{H} , Z and the spectral index Γ . The N_{H} covers $\log(N_{\text{H}}/\text{cm}^{-2}) = 24$ to 25 with steps of $\Delta\log(N_{\text{H}}/\text{cm}^{-2}) = 0.1$. For the metallicity and spectral index the same grid with the previous section was selected; $Z = 0.5, 1.0, 1.5$ and $\Gamma = 1.5, 1.8, 2.4$ respectively.

All three models have been applied to both the *XRISM* and *Athena* simulated spectra. In Fig. 3.12 the simulated spectra along with the best fits and the residuals are presented.

First, for the *XRISM*/Resolve simulated data, when the simple toroidal model is used, the fit shows good statistics with $C\text{-stat}/dof = 1.11$. The values of the input properties retrieved are: $\text{FWHM} = 1297_{-25}^{+3} \text{ km/s}$, $\Gamma = 1.82_{-0.12}^{+0.13}$, $\log(N_{\text{H}}/\text{cm}^{-2}) = 24.62_{-0.03}^{+0.03}$ and $Z = 0.935_{-0.012}^{+0.011}$. It is clear that the toroidal models underestimates the velocity broadening of the line while the column density is slightly larger than the input value, which is a consequence of the BLR that provides an extra layer of absorption. The above suggest potential degeneracies between the properties. .

For the spherical model (green line of Fig. 3.12) the fit gives a relatively accepted $C\text{-stat}/dof = 1.19$. However, the values it returns diverge from the input ones. The velocity broadening is found $\text{FWHM} = 1221_{-28}^{+24} \text{ km/s}$. It fails to constrain successfully the photon index $\Gamma = 1.5_{N/A}^{+0.003}$. Then the spherical medium was found to have $\log(N_{\text{H}}/\text{cm}^{-2}) = 24.28_{-0.01}^{+0.01}$ and $Z = 0.89_{-0.01}^{+0.01}$.

The M6 model (blue line of Fig. 3.12) is the same used in the previous paragraph and therefore the results are summarized as: $C\text{-stat}/dof = 0.96$; $\text{FWHM} = 1338_{-26}^{+27} \text{ km/s}$; $\Gamma = 1.78_{-0.14}^{+0.16}$; $\log(N_{\text{H}}/\text{cm}^{-2}) = 24.49_{-0.05}^{+0.05}$; $Z = 0.995_{-0.018}^{+0.080}$.

Overall, we find that the simple torus models succeeds in constraining Γ and the properties of the torus considering the lack of BLR in this case, but underestimates the broadening. The spherical model, as expected from Section 3.3.3 performs the worst can be ruled out when compared to axisymmetrical geometries like the toroidal models (only torus and full M6 model). While the values of the uncertainties reported here are typically low, it should be taken into account that there are inherent systematic uncertainties associated to our lack of knowledge of the exact geometrical configuration of the circumnuclear material.

In the case of the *Athena*/X-IFU data, the same behavior is reported (see Fig. 3.13), with the

spherical models failing to well reproduce the data. The torus model succeeds in constraining the FWHM and as expected overestimates the N_{H} due to the lack of the BLR. The values derived are: $\text{FWHM} = 1322^{+10}_{-10} \text{ km/s}$, $\Gamma = 2.4^{N/A}_{-0.01}$, $\log(N_{\text{H}}/\text{cm}^{-2}) = 24.66^{+0.01}_{-0.01}$ and $Z = 1.066^{+0.015}_{-0.007}$ for $C\text{-stat}/dof = 1.15$. For the sphere we found: $C\text{-stat}/dof = 1.91$ $\text{FWHM} = 1230^{+10}_{-10} \text{ km/s}$. It fails to constrain the photon index $\Gamma = 1.5^{+0.003}_{N/A}$. Then the spherical medium was found to have $\log(N_{\text{H}}/\text{cm}^{-2}) = 24.76^{+0.01}_{-0.01}$ and $Z = 0.89^{+0.01}_{-0.01}$.

Finally, the M6 model returns the velocity broadening $\text{FWHM} = 1337^{+10}_{-11} \text{ km/s}$, the photon index $\Gamma = 1.75^{+0.04}_{-0.07}$, while the column density is $\log(N_{\text{H}}/\text{cm}^{-2}) = 24.50^{+0.05}_{-0.04}$ and $Z = 0.991^{+0.024}_{-0.008}$, for $C\text{-stat}/dof = 0.96$.

To conclude, we see that with these new, high-resolution data, the spherical geometry (M2 model) can be easily distinguished from the toroidal (M3) and complex AGN model (M6). Nevertheless, the latter two models (M3-torus, M6-complex) show degeneracies between the FWHM, the spectral index and the column density. This finding suggests that the use of the energy range $6 - 8 \text{ keV}$, including the $\text{Fe K}\alpha$ and its CS, has limitation in helping constrain the properties of the circumnuclear material.

3.5 Summary

The Compton shoulder is a feature formed by fluorescent $\text{Fe K}\alpha$ photons that are Compton-scattered to lower energies by the circumnuclear material around the SMBH. Since the CS is result of Compton scattering its shape and flux depends on the physical properties of the medium as well as on the geometry of the system. We have set up a series of simulations, using the ray-tracing platform REFLEX, featuring different physical properties as well as geometries to explore their impact on the $\text{Fe K}\alpha$ CS (for details see Section 3.2). In our main analysis we were focused on the properties of the circumnuclear medium and we decided to keep the inclination angle of the system fixed to the edge-on case ($85^\circ - 90^\circ$). The observing angle is not always known but we consider it an effect related to the orientation between the source and the observer and therefore not a physical property of the medium. However, it can indeed affect the spectral shape and therefore in Section 3.6.4 we explored briefly the effect of it on the $\text{Fe K}\alpha$ and its CS.

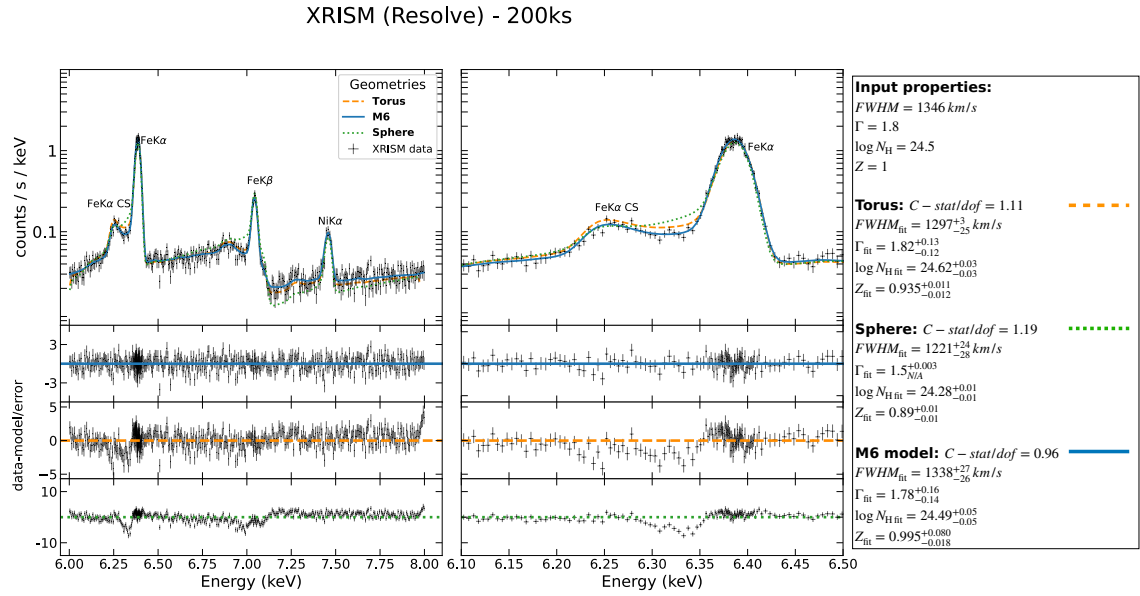


Figure 3.12: The simulated spectra of Circinus around the FeK α line region. The spectra are fitted with a grid model developed using the M6 geometry (see Section 3.3.3) having free parameters the N_H and Z . In the left panel the XRISM/Resolve data along with the data/model ratio are presented. The orange line is the best fit with the retrieved values summarised in the box.

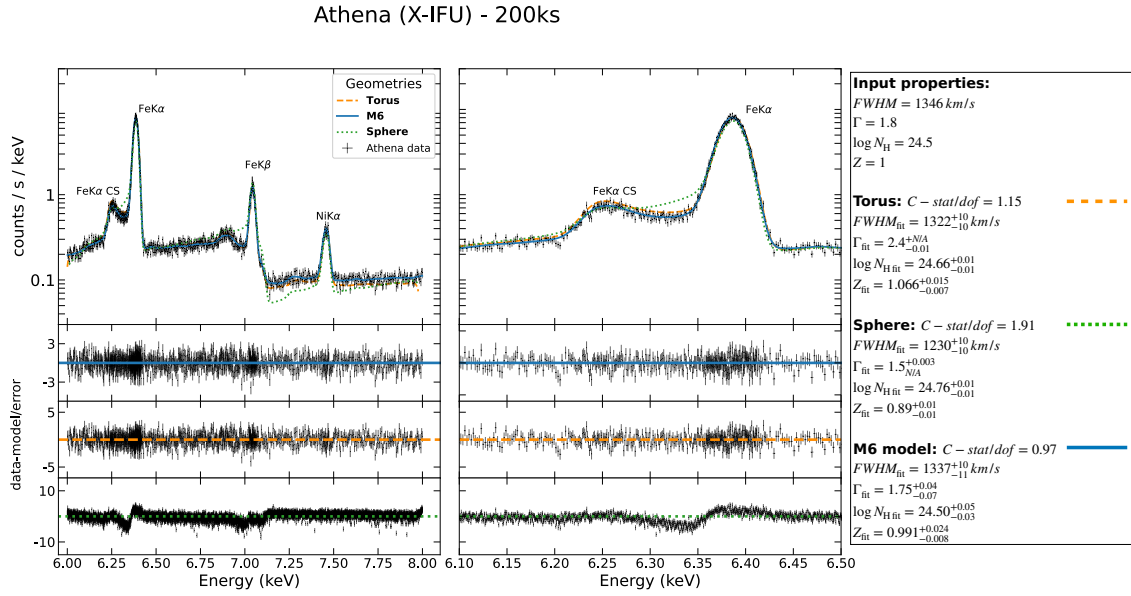


Figure 3.13: The simulated spectra of Circinus around the Fe K α line region. The spectra are fitted with a grid model developed using the M6 geometry (see Section 3.3.3) having free parameters the N_H and Z . In the left panel the *Athena*/X-IFU data along with the data/model ratio are presented. The orange line is the best fit with the retrieved values summarised in the box.

In Section 3.3.1, we present the influence of different physical properties on the CS, whereas in Section 3.3.3 we use different geometries to make complex AGN models with their physical properties fixed. We summarize here our results:

- **Metal composition:** In Section 3.3.1 we tested the three more commonly-used abundance tables that can be found in XSPEC, `angr`, `wilm`, `lodd`.

We found that the behavior of the CS is affected by absorption that is regulated by the use of various abundance tables. Table such as `angr` results in a more prominent shoulder, but the total spectrum suffers from high absorption. On the other hand, when we used `wilm`, `lodd`, which have similar abundance in iron, a less absorbed spectrum with less asymmetrical and thus prominent CS is observed (see Fig. 3.2).

- **Metallicity:** In Section 3.3.1 the metallicity (Z) was tested in order to explore whether it can affect the shape and the flux of the FeK α and its CS. Different values of Z regulate the metals and therefore the absorption of the incident photon field. We tested Z from 0.1 – 2. In Fig. 3.3 as the Z increases, the total flux of the spectrum drops. The flux of the CS also decreases with the metallicity. At high Z (1.5, 2) the shoulder becomes asymmetrical with high peak/bottom ratio (see panels (c), (d) in Fig. 3.3). Our results are in agreement with previous works (e.g., Furui et al. 2016; Odaka et al. 2016).
- **Column density:** In Section 3.3.1 we tested different values of N_{H} ($N_{\text{H}} = 10^{23.5} - 10^{25.5} \text{ cm}^{-2}$). The spectra for the different column densities are presented in Fig. 3.4. Optically thin material is incapable of forming a distinctive CS. On the other hand, high column densities lead to higher absorption, which significantly decreases the overall flux of the CS. The CS shows a characteristic peak at 6.24 keV and becomes more asymmetrical at $N_{\text{H}} \geq 10^{25} \text{ cm}^{-2}$ as shown in in panels (c) and (d) of Fig. 3.4. Previous studies have presented a similar behavior of the CS with varying N_{H} (see, Yaqoob and Murphy 2010, Furui et al. 2016, Odaka et al. 2016).
- **Number of scattering:** In Section 3.3.1 we tested the origin of the photons that form the CS. It has been shown that the CS, for a torus observed edge on, is mostly formed by FeK α photons that have undergone the first four scatterings. For column density

$N_{\text{H}} = 10^{24.0} \text{ cm}^{-2}$ the different scattering events produced mostly symmetrical structures, and we did not observe a significant difference in their shapes. Yet, for high column density $N_{\text{H}} = 10^{25.0} \text{ cm}^{-2}$, the first two scatterings are more asymmetrical than the higher order ones. We explored this further in Fig. 3.6, where we show that the high asymmetry originates from the inner surface of the torus.

- **Dust:** The last physical property tested, in Section 3.3.1, was the presence of dust grains in the torus. The torus extends beyond the sublimation radius and thus, it is expected to be dusty. We tested if the presence of iron on dust grains can change the shape of the CS. To do so, three different *depletion factors* were used; 0, 0.7 and 1.0. We found no significant differences neither to the shape of the CS nor in the fluxes and ratios (see Fig. 3.7).
- **Velocity broadening:** Given that many AGN can feature Fe K α emission line that have been broadened due to GR effects or the motion of the clouds where fluorescence happens, we have applied a gaussian smoothening at 6.4 keV to see whether the CS is diluted by the broadening. Although the kinematics of the circumnuclear material can be very complicated, we have decided to adopt a simple ad-hoc model to show that when any kind of disturbance is applied to the spectrum the CS is highly affected. In Section 3.3.2 are presented the results for four different velocities (0 – 5000 km/s) in two cases of N_{H} of the torus (see Fig 3.8). It is clear that high broadening affect substantially the shape of the CS and therefore there are limitations to the use of the CS as a tool to study the material around the SMBH.
- **Geometries of the circumnuclear material:** In Section 3.3.3 different geometries were used to test the effect of different geometrical components on the shape and the flux of the CS. We created six different models (M1-6) varying from a simple slab reflector to more complex geometries featuring an accretion disk, BLR, torus and a perpendicular hollow cone. Two different observing angles were considered. The edge on view (90°) and mid 45°. We found that the presence of the torus affects the shape of the CS (Models: M3-6), whereas the addition of the BLR (Models: M5-6) adds an extra layer of absorption and therefore affects the flux of the Fe K α and the CS. In the case of the simple slab reflector the flux is found to be lower with no significant contribution, whereas the spher-

ical medium due to its isotropical nature it produces the same results in both observing angles as expected. All the spectra for the different models are illustrated in Fig. 3.9.

In Section 3.4 we used the complex model (M6), which includes the accretion disk, the BLR, the dusty torus and the polar medium (see Fig. 3.1), along with *XRISM* and *Athena* response files to generate simulated spectra for the Circinus galaxy. Velocity broadening of $\text{FWHM} = 1346 \text{ km s}^{-1}$ (Andonie et al. 2022) has been applied to the generated spectra using the `gsmooth` model of XSPEC. Having the simulated spectra for a source that is known to have a $\text{Fe K}\alpha$ Compton shoulder, we were motivated to see whether we can retrieve the input parameters by fitting the CS using a grid model. The M6 model from Section 3.3.3 is used. The properties of all the components except of the torus are fixed to the values of Table 3.2. For the torus, the grid model has free parameters the column density and metallicity. Moreover, the velocity broadening and the spectral slope of the continuum are free to vary too.

Our test is focused on the parameters of the torus and our analysis shows that the model tends to slightly underestimate the FWHM, although the overall fit is good since the model used to generate the simulated spectra and the model used to fit them is the same. (see Section 3.4.1). This is reported for both instruments (see Fig. 3.10 and Fig. 3.11). The motivation was to illustrate the performance of advanced instruments in terms of spectral resolution and seek potential strong degeneracies between the properties.

Next, in Section 3.4.2 we performed another test, this time focused on the geometrical configuration of the system, and whether there are degeneracies between different geometries. We have applied three different models based on three different configurations. The first model is a spherical cloud that surrounds the central source, which performs worse than the other two and suggests that it can be distinguished from the axisymmetric models. When a simple torus along with the M6 model (see Section 3.3.3) are tested the fits gets better. The two models are almost indistinguishable in terms of fit quality. When *XRISM* data are tested the retrieved properties are the same except of the column density which is slightly larger for the simple torus model since it does not include the BLR which contribute to the line-of-sight N_{H} . In the case of the *Athena* spectrum the difference between the fit quality within the two models is larger, although no safe results can be derived from this analysis since the simulated spectra and the grid of the M6 model are identical.

We have shown that the Compton shoulder is a spectral feature sensitive to changes of the circumnuclear material. Its shape is affected by some of the physical properties or the geometry of the reprocessing material. Properties like the metallicity and the column density can have similar effects on the CS, however, they do not affect in a similar way both the Fe K α line and the CS. With the new *XRISM*/Resolve instrument, it will be possible to use the Fe K α CS, along with broadband X-ray spectroscopy, to better constrain the physical properties and geometry of the circumnuclear material around AGN.

Acknowledgements

The authors acknowledge the referees for their useful comments that improved this work. GD acknowledges support from ANID Beca Doctorado Nacional 21211606. CR acknowledges support from the Fondecyt Regular grant 1230345 and ANID BASAL project FB210003.

3.6 Additional tests for the CS shape behavior

3.6.1 Different X-ray sources

Throughout our analysis we used an X-ray input source modeled by a spherical corona, like the lamp-post model, with fixed a fixed power-law with a high energy cutoff (see, Section 2.2.1 for details). However, the geometry of the X-ray source is still under debate, while AGN show a variety of spectral indices as well as energy cutoff (Ricci et al. 2017b). Hence, we performed some tests where the shape of the source deviates from the typical lamp-post to see whether it can affect the Fe K α line and its CS. Moreover, we decided to explore two different spectral indices and check if it is likely to find differences that can be distinguishable.

X-ray source geometry

A spherical corona that resides on top of the SMBH has been used so far, with its properties illustrated in Table 3.1. Here we perform a series of simulations featuring different source geometries. For the reflecting medium a simple toroidal reflector similar to the one used in Section 3.3.1 has been selected, observed edge on. First, we implement a simple point-like

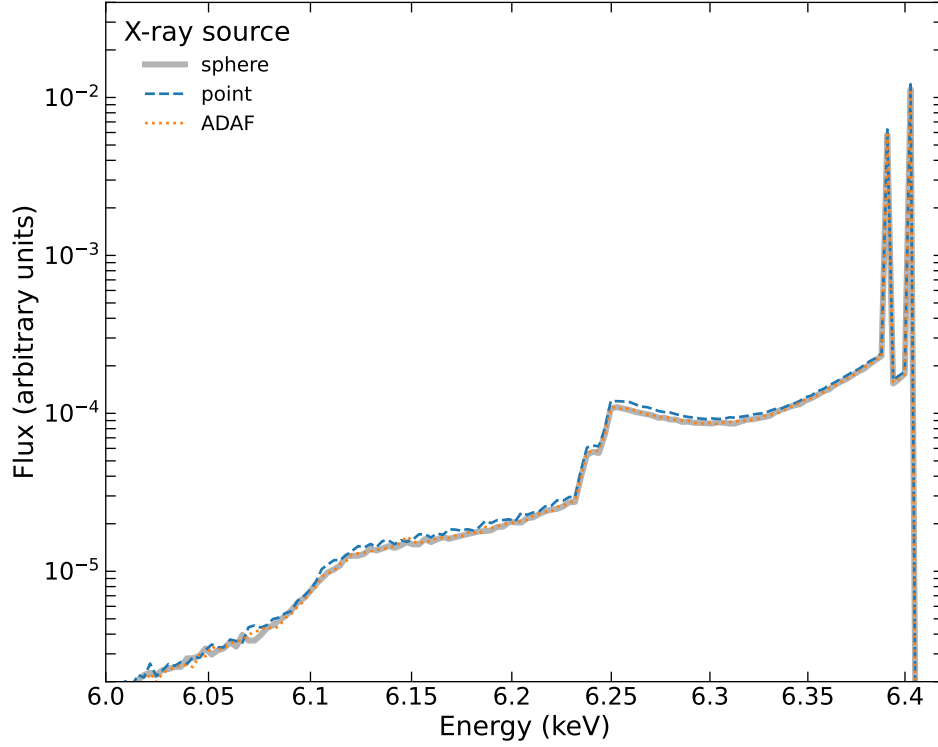


Figure 3.14: The FeK α CS region for different type of X-ray source. Changing the geometry of the input source does not have any effect on the FeK α and its CS as long as the spectral properties remain the same.

source that resides $10r_g$ above the black hole. It emits light in all directions. Next, we change the geometry of the source by adding a sphere that is in the plane of the accretion disk that models an advection-dominated accretion flow (ADAF; [Yuan and Narayan 2014](#)), which can be found in low luminosity AGN. An ADAF-like central source consists of very hot material that starts from radii close to ISCO (Innermost Stable Circular Orbit) and extends up to hundreds of r_g . For our simulations we set center of the sphere in the center of the system and give it $100r_g$ radius, which corresponds to $\sim 1.62 \times 10^{-5}$ pc.

In Fig. 3.14 the Compton shoulder and FeK α line are presented, for the point, the ADAF as well as the spherical corona source. It is clear that the geometry and the position of source do not affect the shape of the CS. We tested the CS ratio for the three different source and the difference is negligible ($< 1\%$). As a result, we suggest that the CS shape is independent of the geometry of the central X-ray source.

X-ray source spectral index

In the simulations we have performed so far, the spectral index of the incident photon field is fixed to $\Gamma = 1.8$, which is common value for AGN (Ricci et al. 2017b). Nevertheless for a given power-law photon distribution any change on the spectral index affects the net amount of photons across the energy space. Since the Fe K α emission line and the corresponding CS span in a very small energy range, we are interested in testing whether a different Γ can produce different shapes of CS. [Yaqoob and Murphy 2010](#) have performed a series of simulations to explore the connection between the spectral index and the shape of the CS. They used a torus with column density $N_{\text{H}} = 1 \times 10^{25} \text{ cm}^{-2}$ and tested two different Γ (1.5 - 2.5) for two observing angles; face-on and edge-on. First, in the face-on regime it is illustrated that the steepness of the of the continuum has a negligible effect on the shape of the CS which in fact makes it non-detectable. However, in the edge-on case the two spectral indices produce distinct spectral shapes of the CS. Flatter spectra provide a larger amount of high energy photons that can penetrate deeper to the torus and therefore are more likely to produce a more symmetrical CS as a result of wider range of scattering angles. On the other hand, steeper spectra ($\Gamma = 2.5$) show a significant back-scattering peak due to the fact that the CS emerges from the back surface of the torus with lesser photons being able to penetrate deep into the medium. [Odaka et al. 2016](#) used a spherical cloud as circumnuclear medium, featuring column density $N_{\text{H}} = 1 \times 10^{24} \text{ cm}^{-2}$ and metallicity $Z = 1$, to test a variety of spectral indices (1.2 – 2.8). For the tested column density they did not find any particular difference in the shape of the Fe K α and the CS. They report that the equivalent width of both features ($EW_{\text{FeK}\alpha}$, EW_{CS}) show an anti-correlation with the photon index, which suggests that Γ affects the production of fluorescent photons and not the shape of the CS, which is the outcome of scatterings. However, the column density they tested it might not be enough for the CS to show a difference in its shape for steeper and flatter continua. We decided to apply a similar exercise by testing two opposite scenarios of Γ in two tori with high column densities ($\log(N_{\text{H}}/\text{cm}^{-2}) = 25.0 - 25.5$). The spectra are collected for edge-on observing angles, since it has already been shown that for face-on angles the effect is negligible. The properties of the torus are fixed to the properties presented in Section 2.2.1. In Fig. 3.15 two panels are presented for the two different column densities. In both cases are

illustrated the spectra in the Fe K α energy region for a soft continuum ($\Gamma = 2.4$, solid line) and a hard one ($\Gamma = 1.5$, dashed line). For $\Gamma = 1.5$ in both panels it is clear that the total flux of the Fe K α and the CS is higher than $\Gamma = 2.4$ due to the larger amount of photons that can cause fluorescence. Considering the shape of the CS, we do not observe any significant variations in none of the two cases tested, suggesting that the formation of more or less Fe K α photons dominates any scattering process. Therefore, the Compton shoulder cannot be a reliable feature to constrain neither the geometry nor the spectral index of the X-ray source since they do not have a strong effect on it.

3.6.2 The Broad Line Region

In Fig. 3.1 a schematic of all the components, used, is presented. The broad line region (BLR) has been modeled as a flared disk; a disk with increasing z-axis height as we move across its radius. In order to build the flared disk we used a combination of blocks one on top of each other, with decreasing radial length. To test the efficiency of this method we test BLR models that consist of 10, 20 and 30 blocks. The cubic density was fixed in all blocks (see Table 3.2). In Fig. 3.16 the spectra for different number of blocks are illustrated. In case of 10 blocks the total flux of the Fe K α and its CS is low. On the other hand, when the BLR consists of 20 and 30 blocks the difference is negligible. Consequently, we decided to use 20 blocks in the rest of our work, a number that saves computational time and provides good resolution.

3.6.3 H₂ Fraction

Another physical parameter tested is the molecular hydrogen percentage in the circumnuclear material (H_2 fraction). By tuning the H_2 option in our simulations we can change the percentage of H_2 that is present in the reprocessing medium. We set four different simulations, increasing H_2 ; i) 0, ii) 0.2, iii) 0.5, iv) 1.0 using a torus with the default settings presented in Table 3.2. In Fig. 3.17 the spectra of the simulations are presented. We can see that the H_2 percentage does not affect the shape of the CS in any way. [Sunyaev and Churazov \(1996\)](#) have shown that molecular hydrogen and helium interact mostly elastically with X-ray photons, and therefore they do not affect the Compton shoulder.

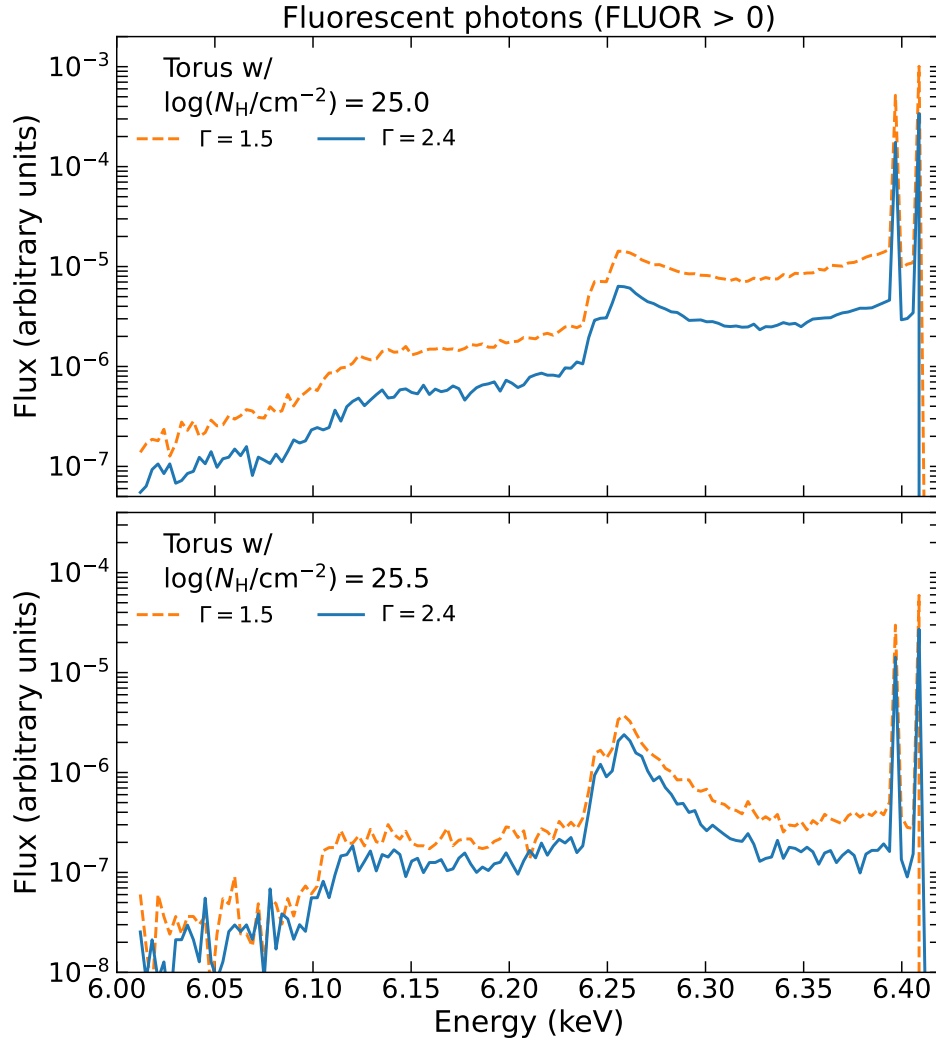


Figure 3.15: The FeK α CS region for two different intercepting tori *Top*: Column density $N_{\text{H}} = 10^{25.0} \text{ cm}^{-2}$, *Bottom*: $N_{\text{H}} = 10^{25.5} \text{ cm}^{-2}$. Two opposite scenarios of spectral indices of the X-ray source have been tested. One flatter spectrum (1.5) and one steeper (2.4), which for a given distribution can affect the net amount of photons available near the K-edge. Only photons that originate in fluorescence are considered.

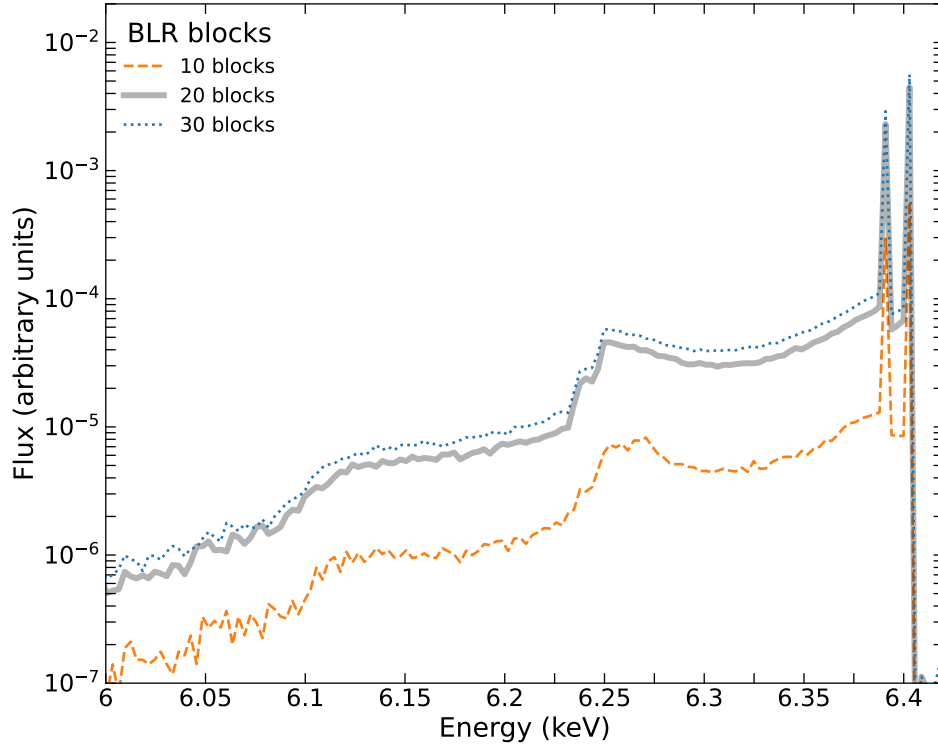


Figure 3.16: The CS spectral region for BLR consisting of different number of building blocks. Higher complexity increases the computational time of our simulations and therefore we select 20 blocks that provide sufficient photons while keeping the simulations in reasonable running times.

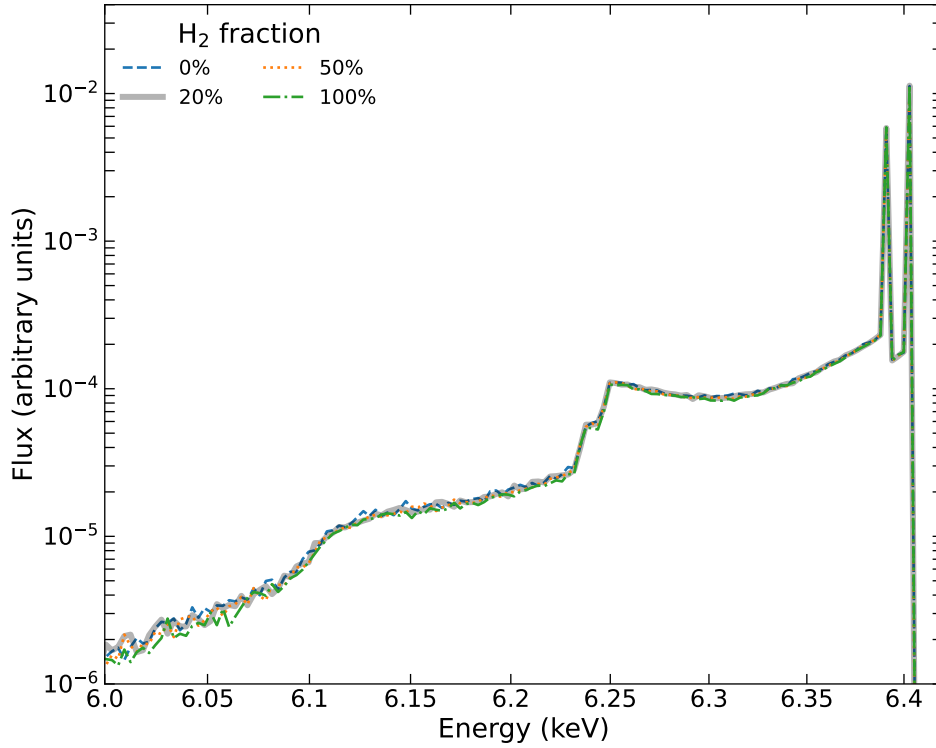


Figure 3.17: The Fe K α CS spectral region for different H₂ fractions. The amount of molecular hydrogen in the circumnuclear material has no effect on the CS and the Fe K α line.

3.6.4 Inclination angle

The main analysis of this work is focused on the circumnuclear material and how its physical properties or geometrical configuration can affect the Fe K α and its corresponding Compton shoulder. Hence, the observing angle, a property that it is an effect that it is related to the relative orientation between the observer and the source has not been explored in detail (except of Fig. 3.9). Nevertheless it is known that that various observing angles can indeed produce different CS shapes. Since not all AGN are observed edge on, we test how the Fe K α and CS vary with the observing angle. [Odaka et al. \(2016\)](#) used a slab geometry reflector with an X-ray source above it. They collect the spectrum from 5 different angle bins ($0^\circ - 10^\circ$, $20^\circ - 30^\circ$, $40^\circ - 50^\circ$, $60^\circ - 70^\circ$, $80^\circ - 90^\circ$). In angles $\geq 20^\circ$ the shape of the shoulder is relatively the same. In the face-on regime there is a peak at ~ 6.32 keV, which corresponds to a scattering angle of 90° .

In our simulations, we build a simple model that includes an X-ray source (see Table 3.1 and a slab reflector (disk in Table 3.2). To focus only on the Fe K α line and its corresponding CS, we collect photons that come from fluorescence and have been scattered only once (SCATT == 1). We have performed 4 different simulations collecting photons in different angles covering from face-on to edge-on scenario. In Fig. 3.18 the Fe K α and CS region is shown. Our results are in agreement with [Odaka et al. \(2016\)](#) and illustrate the dominant scattering angle in each case and, consequently, the amount of energy a fluorescent photon loses after its first Compton scattering.

Having tested how the shape of the CS changes in the case of a slab reflector, we proceed to test different observing angles for more complex geometries. To do so, we use the M6 model presented in Section 3.3.3 which includes all of the components from Table 3.2. We set three different inclination angles for the simulations; 30° , 60° , 90° (5° bin). In Fig. 3.19 the spectra are presented in the Fe K α energy region.

In panel (a) of Fig. 3.19 it is shown that the total flux drops with the angle as a result of the absorption. Moreover, the shape of the CS changes, too. Low inclination angles produce a much flatter CS, which can be related to the previous simulation where the disk in low angles enhance the shoulder. The shoulder becomes asymmetrical for 60° and then returns to a more

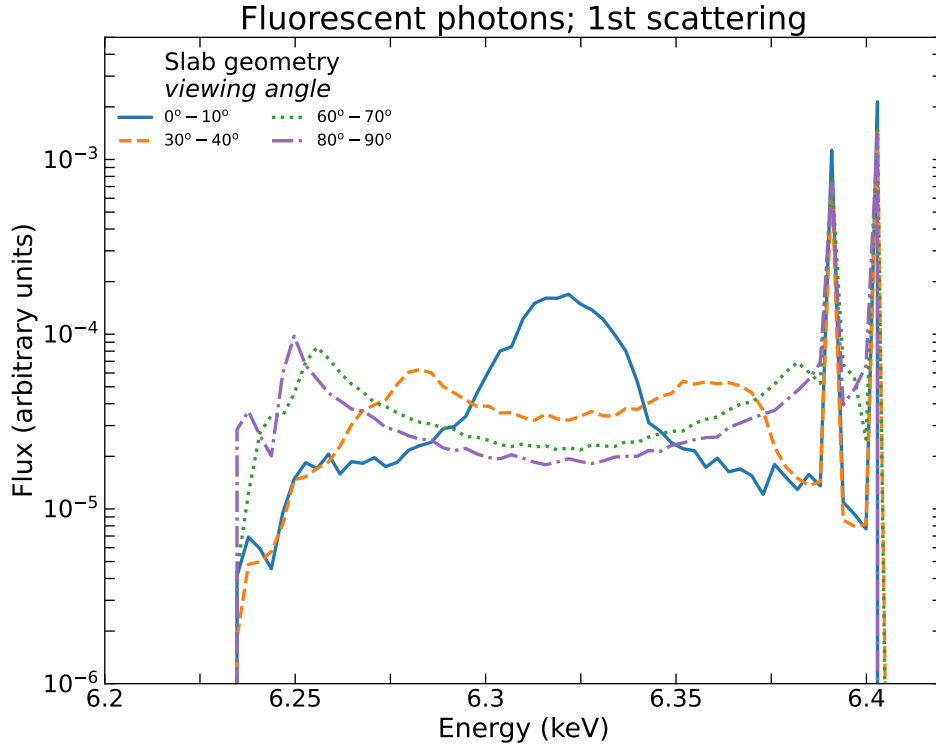


Figure 3.18: *Top*: Spectra in the range of the Fe K α line and its CS for a slab reflector observed in different angles. The spectra illustrate photons that originate from fluorescence and have undergone one scattering.

symmetrical profile (see panel (c) of Fig. 3.19). At the same time, the peak at 6.24 keV becomes more apparent as the angle increases. In Fig 3.19 panel (d) the peak/bottom ratio shows a positive trend.

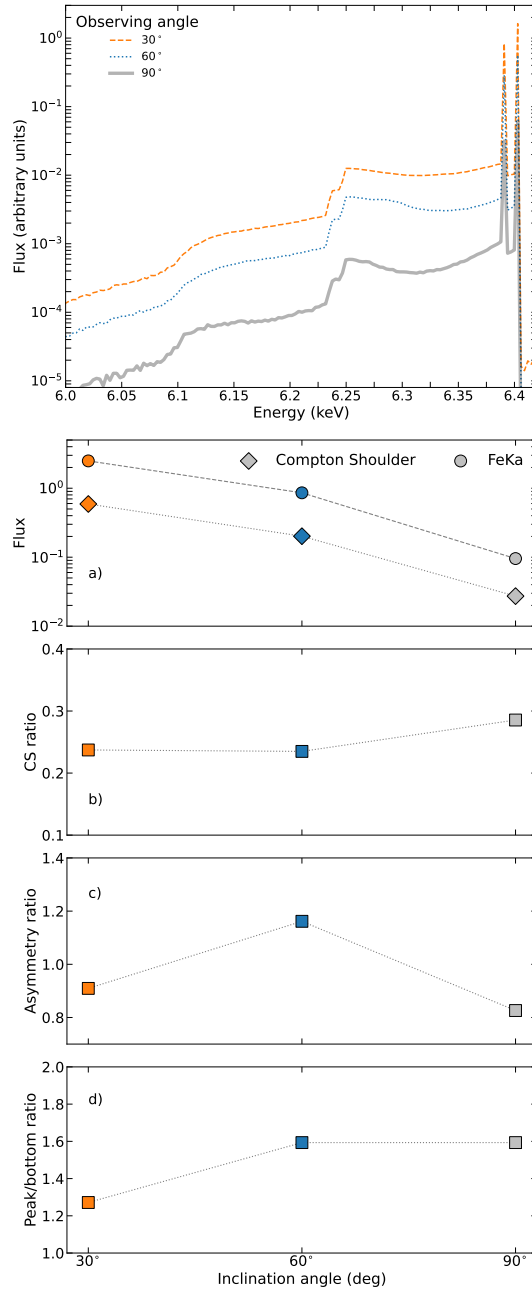


Figure 3.19: *Top*: The AGN model (M6) observed in different inclination angles. *Bottom*: a) The CS and FeK α flux, b) The ratio of the CS flux and the FeK α line, c) The asymmetry ratio and d) peak/bottom ratio. The colors represent the column densities introduced in the top panel.

Chapter 4

X-GATOS

The following chapter reports on the application of newly built X-ray spectral models on Seyfert galaxy NGC 4941. The idea is that we can use the flexibility of REFLEX to build an X-ray spectral model based on the physical and geometric properties recovered by multi-wavelength studies of the source. At this stage, we provide an analysis of one source, but this project will be expanded to four sources from the GATOS survey ([García-Burillo et al. 2021](#); [Alonso-Herrero et al. 2021](#)).

4.1 Introduction

Disentangling the properties of the material around the SMBH is crucial to understanding AGN physics. However, this task can be challenging because of the small angular size of these structures and the typical distances of the sources, where emission from the host galaxy often dominates in most bands. However, with the development of modern facilities and instruments, the necessary angular resolution has now reached levels that, for local sources, allow us to resolve material close to the nucleus and thereby put the Unified Model under scrutiny ([Tristram et al. 2007, 2009, 2014](#); [García-Burillo et al. 2016](#); [Izumi et al. 2018](#); [GRAVITY Collaboration et al. 2020b](#); [López-Gonzaga and Jaffe 2016](#), see also reviews [Netzer 2015](#); [Ramos Almeida and Ricci 2017](#); [Spinoglio and Fernández-Ontiveros 2019](#)).

The Galaxy Activity, Torus, and Outflow Survey (GATOS) is a project that aims to thoroughly study a selection of local Seyfert galaxies by investigating the properties of the mate-

rial surrounding the central AGN and its connection to the host galaxy. The core sample of GATOS consists of 19 sources that span a wide range of luminosities, Eddington ratios, and obscuration levels (García-Burillo et al. 2021, hereafter GB21). The GATOS targets benefit from multiwavelength observations, from X-ray to radio, allowing better constraints on both the properties and the behavior of the central AGN.

In GB21, the authors used ALMA observations to study the cold neutral material around the SMBH on scales from a few parsecs to several kiloparsecs. In particular, they traced the CO(3-2) and HCO⁺(4 – 3) molecular emission lines, as well as the submillimeter continuum (370 μ m $\sim$ 351 GHz), at a spatial resolution of 0.1'' ($\sim$ 7 – 13, pc). They found that all sources host a circumnuclear disk/molecular torus¹ with a median diameter of 42 pc.

Twelve sources from the GATOS sample have been observed in the mid-IR and far-IR (Alonso-Herrero et al. 2021, hereafter AH21). Half of these showed prominent mid-IR emission oriented perpendicular to the disk seen in ALMA (GB21), suggesting that the mid-IR emission arises along a polar direction and possibly connects to the more distant narrow line region (NLR). The CAT3D-WIND radiative transfer models (Hönig and Kishimoto 2017), which include model images at 8 μ m, 12 μ m, and 700 μ m, were built in order to get applied on these observations. They feature various configurations, including compact and extended configurations for the disk and wind, "thin" and "thick" geometries for the disk and cone walls, and a range of wind-to-disk ratios. Most galaxies in the sample with extended mid-IR emission show intermediate-to-high nuclear column densities ($\log N_{\text{H}}(\text{ALMA}) \sim 22.5 - 23.9 \text{ cm}^{-2}$) and moderate Eddington ratios ($\log \lambda_{\text{Edd}} \sim -1.9$ to -1.2), with $L_{2-10\text{keV}} > 1.5 \times 10^{42} \text{ erg s}^{-1}$. According to simulations by Venanzi et al. 2020, these conditions are necessary to launch dusty winds.

From the broader GATOS sample, we selected for this study NGC 4941, a galaxy that exhibits high column density $> 10^{23} \text{ cm}^{-2}$ (Ricci et al. 2017a) and has multiwavelength observations that can help us build a tailor-made model in the X-ray band. Some extra sources that share similar characteristics, and which will be studied in a future work, are NGC 7582,

¹Even though the exact geometry of the circumnuclear disk or torus is under debate, in this work we use the term "torus" to refer to the dusty, molecular structure that is roughly parallel to the SMBH's plane of rotation, so as to distinguish it from material located outside the black hole's dynamical boundaries.

NGC 4388, and NGC 5643. These galaxies exhibit high column densities ($N_{\text{H}} > 10^{23.5} \text{ cm}^{-2}$; Ricci et al. 2017a) and are therefore classified as obscured, showing strong reflection features in their X-ray spectra. NGC 1068 and the Circinus galaxy are also well-known obscured sources in the GATOS sample. However, because they have already been studied extensively in the past, we do not include them in this work (e.g., Tristram et al. 2007, 2014; Izumi et al. 2018; Stalevski et al. 2017; Stalevski et al. 2019; Jaffe et al. 2004; López-Gonzaga et al. 2014; GRAVITY Collaboration et al. 2020b).

The aim of this work is to explore what properties can be retrieved from the X-ray spectra of these sources by using the ray-tracing code REFLEX (Paltani and Ricci 2017; Ricci and Paltani 2023). We build the models for NGC 4941 that include the structures found in the GATOS studies, such as the circumnuclear disk/torus and the polar wind, and we investigate the potential synergy between the X-ray and sub-mm/IR observations in model building.

4.2 Targets

4.2.1 NGC 4941

NGC 4941 is a Seyfert II galaxy (Véron-Cetty and Véron 2006) that was observed from the ASCA observatory in 1996 and 1997 (Terashima et al. 2002) and *BeppoSAX* in 1997 (Maiolino et al. 1998), where the obscure nature of the source with a strong FeK α was revealed. The black hole mass of NGC 4941 is estimated to be $\log M_{\text{BH}}/M_{\odot} \approx 7.03$ (Koss et al. 2017), and the X-ray luminosity $L_{2-10\text{keV}} = 1.98 \times 10^{41} \text{ erg/s}$ places it in the *low-luminosity* category of AGN. A recent study from Kawamuro et al. (2013), using *Suzaku* and *Swift*/BAT data, suggests that NGC 4941 is an obscured source that has an inclination angle of 70° , featuring a moderate covering factor of around 0.3-0.5.

Observations of molecular gas in NGC 4941 using the CO(3-2) line show a twin peak morphology within a radius of 50 pc. There is less molecular gas at the AGN location. The two CO peaks have a "butterfly" shape and are located symmetrically around the AGN along a position angle of about 40° . The central AGN is also surrounded by continuum emission as observed with ALMA at 351 GHz. This central emission is due to the presence of dust and is

elongated along the same position angle as the CO peaks. However, as reported in GB21 the extended polar emission of 351 GHz coincides with the outflow orientation found by Barbosa et al. 2009. Hence, the polar emission is believed to be associated with outflow and not with polar dust emission, since NGC 4941 is a low luminosity AGN and cannot generate strong winds (see also AH21 and Venanzi et al. 2020).

For NGC 4941 we used a series of geometrical objects available in REFLEX. To scale the components when needed we used the $M_{\text{BH}}/M_{\odot} = 7.03$, and the X-ray luminosity $L_{2-10\text{keV}} = 1.98 \times 10^{41} \text{ erg/s}$.

As expected, the first component is the X-ray source that is placed above the SMBH in the simulation box. The black hole is not a physical component in our models since the code does not reproduce GR effects on the X-ray radiation. Yet, we consider the very center to be the "black hole", which is handy in order to place and orientate the rest of the components. The X-ray source is a SPHERE that is placed at 10 Schwarzschild radii (r_g) above the center, where r_g is the gravitational radius of the black hole and is defined as $r_g = 2GM_{\text{BH}}/c^2$. The radius of the sphere is set to $6 r_g$. These values follow well established measurements of reverberation of X-ray on AGN. However, the exact shape and whether there is a unique population of electrons in the corona are still under debate. The X-ray source "emits" a power-law spectrum with a photon index Γ and a cutoff energy at 200 keV. The photon index is a free parameter and varies from 1.6 to 2.4 with a step of 0.1. Since we have available data from Chandra and NuSTAR, the source generates photons from 0.3 to 100 keV. In terms of the collected spectra, they are divided into two categories. The soft part (0.3–10 keV) is binned with a spectral resolution of 50 eV and the hard part (10–100 keV) is binned with a logarithmic step of 0.01. Our motivation lies on the fact that we are using CCD data from the *XIS* instruments onboard the Suzaku mission, which do not exceed 70 eV spectral resolution in any energy range. As a result, both resolutions were chosen to match the available data and to keep computational time at a reasonable level. The observing angle is a free parameter and varies from 0 to 90 degrees with a step of 10 degrees.

For the accretion disk, we use the ANNULUS object from the library of geometries found in REFLEX. We set the hydrogen to be ionized using TEMPERATURE 1 and consequently, the molecular hydrogen is absent (H_2 FRACTION 0). Moreover, the metal composition is set to MATTER lpg (Lodders et al. 2009) with the default metallicity unity (METALLICITY 1) and, as

expected, there is no dust in the accretion disk (DUST 0). In terms of scaling, our accretion disk starts at $10r_g$ and extends up to $\sim 1000r_g$, a value that we consider reasonable based on reverberation studies of the accretion disk (McHardy et al. 2023). The optically-thick accretion disk model is thought to have Thomson optical depth $\tau > 100$ which results in column densities $N_H \sim 10^{26} \text{ cm}^{-2}$. Applying these values to our scaled accretion disk yields a volumetric density of $n \sim 10^{14-15} \text{ cm}^{-3}$. In our simulation, we use $n = 10^{14} \text{ cm}^{-3}$.

The accretion disk is thought to be fed by the BLR (see, Section 1.1.4). Although, the BLR has not been directly observed in NGC 4941, it should be the physical link between the outer dusty medium and the accretion disk. For this reason, we model the BLR as a flared disk (GRAVITY Collaboration et al. 2024b) that starts after the accretion disk and extends up to the sublimation zone following a logarithmic increase in height. This geometry is modeled using a series of annuli (30 blocks). Regarding the physical properties of the BLR, we adopt the same properties as those of the disk above. The next step is to define the size of the BLR and its density. The outer boundary as mentioned above is the sublimation zone which is calculated for a given bolometric luminosity (L_{bol}) using the relation reported by Mor et al. (2009):

$$R_{\text{sub}} = 1.3 L_{46}^{0.5} \times \left(\frac{1500\text{K}}{T_{\text{sub}}} \right)^{2.6} \text{ pc} \quad (4.1)$$

where R_{sub} and T_{sub} are the sublimation radius and temperature, respectively, while $L_{46} = L_{\text{bol}}/10^{46} \text{ erg s}^{-1}$. We adopted the 2 – 10 keV luminosity of NGC 4941 $L_{2-10} = 1.98 \times 10^{41} \text{ erg s}^{-1}$, (Ricci et al. 2017a), and converted the X-ray luminosity to bolometric using as bolometric correction $\kappa = 20$ (Vasudevan and Fabian 2009). In this case, the sublimation zone extends up to $\approx 52.4 \text{ ld}$.

The main novelty of this model is the modeling of a flexible BLR that has two free parameters in the model. The first free parameter is the line-of-sight column density, which has been set to vary. We generate a logarithmic parameter space that starts from $10^{22.0} \text{ cm}^{-2}$ and increases to $10^{25.5} \text{ cm}^{-2}$, having 10 steps. These values are calculated across the line-of-sight at 90° . The BLR we developed varies in terms of size. We consider 4 different setups that cover a range of opening angles (opening angle is defined as the angle from the plane of the SMBH towards the zenith). Our BLR has opening angle $\theta_o = 20, 40, 60, 80$ degrees. This angle is used to calculate the physical size of the BLR since it is known to extend up to the sublimation

zone but its height is unknown. The ratio of the BLR height to the sublimation radius, $\frac{H_{\text{BLR}}}{R_{\text{sub}}}$, corresponds to $\tan(\theta_o)$. These are the only free parameters of the model that are related to the obscuring medium.

The BLR as mentioned above terminates at the sublimation zone and it is continuously connected to the dusty torus (see Section 1.1.5). For this component, we set the same metal composition to be consistent with the previous components (MATTER lpgs). The METALLICITY is set to unity. The torus is dusty and therefore we set $\text{DUST} = 1$, which means that all iron atoms are in dust grains (for more details see Ricci and Paltani 2023). We assume that H_2 FRACTION is 30%. The outer boundary of the torus is at 39 pc (see, AH21). The density of the torus is also set by the ALMA measurements of N_{H_2} which for NGC 4941 is $\sim 10^{21.9} \text{ cm}^{-2}$. To do that, they integrated the CO inside the region covered by the ALMA FOV and assumed 3–2/1–0 brightness temperature ratio ~ 0.7 . Also, a Milky-Way CO-to- H_2 conversion factor was used ($X_{\text{CO}} = 2 \times 10^{20}$) (more details in GB21).

4.3 Observations and model code

4.3.1 Observations

Our study is focused on the X-ray band, and therefore observations from X-ray observatories were used exclusively. For NGC 4941 we used the *Suzaku* observation with Obs ID 707001010, (observed and analyzed by Kawamuro et al. (2013)) and the *NuSTAR* observation with Obs ID 60061236002. NGC 4941 has not shown significant variability, and therefore the time difference between the observations is not expected to affect the results. Details are in Table 4.1.

For data reduction and spectral extraction, we used three different software packages depending on the instrument. For the *NuSTAR* data we used the *NuSTARDAS* software package version 1.9.2 (Nasa High Energy Astrophysics Science Archive Research Center (Heasarc) 2014). We used the standard *nupipeline* script to extract the spectra from the source and the background. We set the radius of the source region to $50''$ and the background region to be an annulus with an inner radius of $60''$ and an outer radius of $90''$. The *XIS-13* spectra *Suzaku* have been obtained from Kawamuro et al. (2013).

In order to build the X-ray spectral model we used the ray-tracing code REFLEX (Paltani and Ricci 2017; Ricci and Paltani 2023), which has been presented in previous chapters of this thesis in detail (see, Section 1.3)

Table 4.1: The observations of NGC 4941 as well as the rest of the GATOS sources that will be studied.

Name	Observatory	Obs ID	Date	Exposure time (s)
NGC 4941	Suzaku	707001010	2012-06-22	80859
	NuSTAR	60061236002	2016-01-19	20664
NGC 4388	NuSTAR	60501018002	2019-12-25	50360
	XMM-Newton	852380101	2019-12-25	74000
NGC 7582	NuSTAR	60201003002	2016-04-28	48488
	XMM-Newton	0782720301-	2016-04-28	101200
NGC 5643	NuSTAR	60061362006	2020-03-26	48104
	XMM-Newton	0601420101	2009-07-25	54520

4.4 Spectral fitting and results

For the spectral fitting of NGC 4941 we used the X-ray analysis software XSPEC version 12.15.0. We use an additive table model from the simulation grid described in the previous paragraph (see for details 4.2.1). In fact we break the model we use into two components. The first is the *int* and the second *cnt*, which consider the reprocessed part (interacting photons) and the continuum part, respectively. Moreover, we used the TBABS model (Wilms et al. 2000) to account for Galactic absorption, which has been set to $N_H = 2.25 \times 10^{20} \text{ cm}^{-2}$ (HI4PI Collaboration et al. 2016). In XSPEC notation the model is written as:

$$model = tbabs \times (ngc4941_{int} + ngc4941_{cnt}) \quad (4.2)$$

where $ngc4941_{\text{component}}$ is the name of the model that was built for this particular source.. We used χ^2 statistics after ensuring that each of our energy bins contains at least 25 counts. This has been applied to both the *Suzaku* and *NuSTAR* data. The fit delivers $\chi^2/d.o.f =$

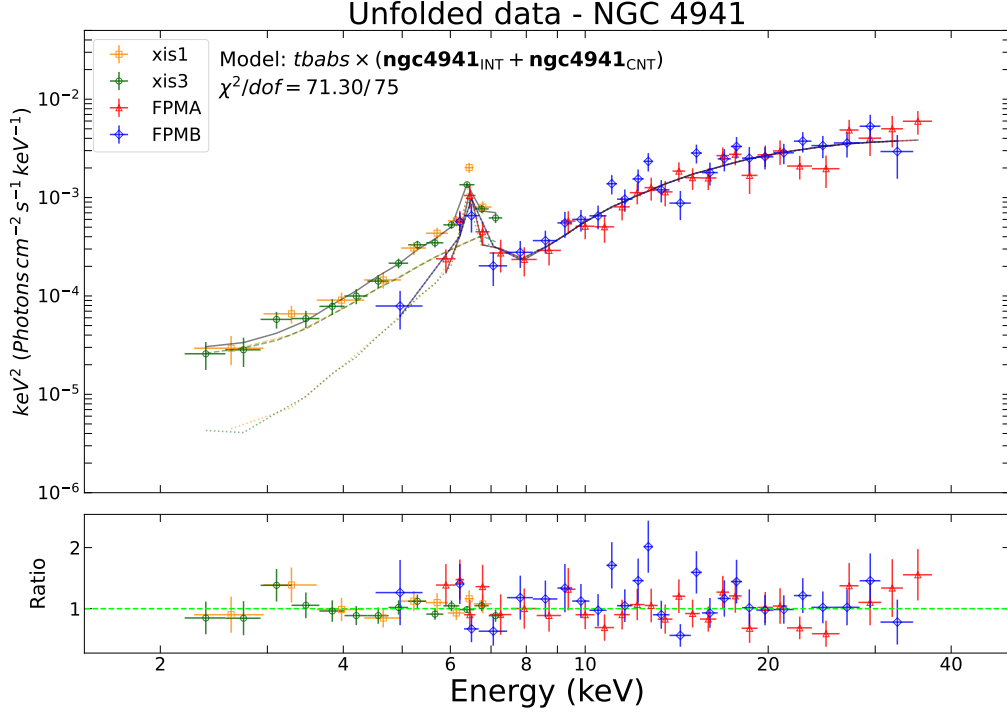


Figure 4.1: The best fit model for NGC 4941. The top panel shows the unfolded data and the model components, while the bottom panel shows the ratio between data and the model.

71.30/75. All errors reported are presented in 90% confidence level and they were calculated from MCMC chains. The observing angle is found to be $\theta = 75.00^{+9.81}_{-9.88}$, while the photon index of the source is $\Gamma = 2.18^{+0.22}_{-0.48}$. The properties of the BLR are found to be $\log(N_{\text{H}}/\text{cm}^{-2}) = 22.79^{+2.71}_{-0.79}$ and the opening angle $\phi_{\text{BLR}} = 59.95^{+11.56}_{-18.93}$. The normalization of the reprocessed part of the radiation is $norm_{\text{repro}} = 9.91 \times 10^{-6}$ while the value for the continuum is $norm_{\text{repro}} = 6.18 \times 10^{-6}$ for the *Suzaku* dataset. We let the continuum of the *NuSTAR* spectra unlinked to take into account potential variability, but the spectrum in the hard X-rays is dominated by reflection and the $norm$ was negligible ($\sim 10^{-22}$). In Fig. 4.1 we show unfolded data along with the model components, as well as the ratio between them.

These results are preliminary and the spectral fitting of the source will continue with other models to further explore the degeneracies and better understand the effect of the geometries on the retrieved values. However, during the spectral fitting and the test we performed, as well as the MCMC chains we ran, we never retrieved high column density for the BLR, or at least combined with the gigantic torus, whose effect at least in the line of sight is negligible (order

of magnitude 10^{21} cm^{-2}). What makes a big difference is the presence of three components, disk–BLR–torus, that all together seem to contribute significantly to the reflection of the spectrum and therefore the total line-of-sight column density remains significantly lower than the literature ($> 10^{23} \text{ cm}^{-2}$, (Kawamuro et al. 2013; Ricci et al. 2017a; García-Burillo et al. 2021)). The column density retrieved from the fit has high errors that can go up to the Compton thick regime, and hence such a case should not be neglected. The use of realistic geometries opens a new window in the X-ray spectral fitting. We need to be cautious, but the momentum given the multiwavelength studies is promising and the data from more advanced instruments such as *Resolve* will nudge the community towards advanced modeling.

Chapter 5

Final remarks

The four-year doctorate program and the projects that have been developed throughout these years have been summarized in this thesis. However, the total work needed cannot be summarized in one document, since obstacles and setbacks have been a major part of the learning process. The following sections summarize the main contributions of this work, the conclusions that can be drawn from the work done, and the steps that can evolve this work further.

5.1 Conclusion

It is clear that the black holes that started as imaginary black stars in the 18th century have become a reality in the 21st century. Stronger than ever evidence, like direct imaging of supermassive black holes, has established the study of them as a major field in astrophysics. The study of supermassive black holes in the center of galaxies is linked to the study of the material that surrounds them. This very material is the one that feeds them and eventually makes them grow to gigantic scales. In this PhD, my role was to take the lead from the current modeling of the circumnuclear material, improve it, and make it more realistic. The X-ray spectrum has become the preferred tool for examining the core regions of AGN. This is primarily because X-ray photons are universally emitted by AGN, and it requires extremely high densities to diminish their visibility in this band. Nevertheless, X-ray spectral modeling has been mostly focused on simple geometries such as slabs and tori, although advancements in other wavelengths support that the medium is organized in various and more complex configurations, putting the unified

model in jeopardy.

The first part of this thesis (Chapter 2) presents the development of a new X-ray spectral model that takes into account the complexity of the circumnuclear material. We used ray-tracing simulation to make two new table models, RXTOP and RXAGN1, that are publicly available and introduce the new era of X-ray spectral modeling, suitable to high quality spectra from microcalorimeters such as the *Resolve* instrument on board the *XRISM* mission.

Next, we decided to specifically focus on the FeK α line and the corresponding Compton shoulder. In this project, we examined how the various physical properties and geometries of the circumnuclear material affect the FeK α line and the Compton shoulder in terms of flux, shape, and relative intensity between them. We claim that such a fine spectral feature is sensitive to changes in the intercepting material and therefore it can be used to put constraints on the geometry and physical properties of the circumnuclear material.

The final project, presented in Chapter 4, illustrates the power of ray-tracing codes like REFLEX in the development of tailor-made models for specific sources. We used the geometrical constraints for NGC 4941 put by submillimeter and IR observations as part of the GATOS survey, in order to make an X-ray spectral model that implements the suggested geometries. The potential of such exercise is high and it is part of the final project to make models for more sources such as NGC 7582, NGC 4388 and NGC 5643.

Overall, this doctorate has been a great learning experience, not only in the field of X-ray spectral modeling but also in the field of AGN and the circumnuclear material in general. From technical skills to understanding of the physics behind the models, I have learned a lot and I am looking forward to continuing to learn and improve my skills in the future.

5.2 Future work

The study of the AGN, the physical mechanism that governs these astrophysical objects, the theoretical framework, and the observations do not stop there. The work done has put the foundations for me to continue working in this field and explore new ideas that can help in the future to better constrain the properties of the SMBH and the material that surrounds them. However, if someone would ask what the main direction is that the current work can take, I

would say that the following four are the most promising:

- **The FeK α line and the Compton shoulder:** The work done in Chapter 3 is a first step to understand the FeK α line and the Compton shoulder. The next step would be to use the models developed in this thesis to fit high-resolution spectra from the *XRISM* observatory and put constraints on the circumnuclear material.
- **The GATOS survey:** The work done in Chapter 4 is a first step to understand the circumnuclear material in NGC 4941. The next step would be to make tailor-made models for more sources that are nearby and there are plenty of multiwavelength observations. A potential option to expand to, is the domain of interferometry that can provide even finer details of the circumnuclear medium.
- **The ray-tracing code:** The work done in Chapter 2 is a first step to understand the ray-tracing code and its potential. The next step would be to use the code to develop new models that can implement different physical conditions for the media, or even new physical processes like kinematics or X-ray sources with various spectral distributions.
- **The BASS survey:** The models RXTOP0 and RXAGN1 have been introduced in this thesis and are publicly available. The next step would be to use them to fit the spectra of the BASS survey and put constraints on a large sample of AGN. In this way we will be able to have some large-number statistics about the geometry of AGN for the first time.

All of the above are just some initial ideas that can generate even more ideas and projects. The flexibility of the current PhD project allows me to branch out and explore various possibilities. The work done on this thesis is just the beginning of a long journey that I am eager to take.

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