Ionised outflows and multi-wavelength variability of Active Galactic Nuclei

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I, Missagh Mehdipour, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.
Abstract

This thesis presents a study of ionised outflows and multi-wavelength variability of Active Galactic Nuclei (AGN) focusing on three Seyfert-type objects: NGC 3516, Mrk 509 and ESO 113-G010. For this work I have made use of mostly XMM-Newton data, i.e. high-resolution X-ray spectra from the Reflection Grating Spectrometer (RGS) for exploring the ionised outflows, and simultaneous optical/UV/X-ray data from the Optical Monitor (OM) and the European Photon Imaging Camera (EPIC) instruments to study the intrinsic emission and variability.

I have investigated the structure and geometry of the partial-covering multi-phase ionised absorber of NGC 3516. I demonstrate that the X-ray variability, originally attributed to occultation by a cloud in an accretion disc wind passing in front of the source, is rather the result of changes in the intrinsic emission of the source. From a 100-day multi-wavelength campaign on Mrk 509, I find that the character of its variability, strictly correlated in the UV and soft X-ray bands, indicates that the soft X-ray excess emission is produced by Compton reprocessing of the UV disc emission in a warm corona encasing the inner disc. I have also studied the nuclear obscuration and the role of dust in the warm absorber of ESO 113-G010. I show that the cause of significant optical/UV reddening, despite the lack of X-ray absorption from neutral gas, is most likely to be dust embedded in a weakly-ionised phase of an absorber which is conspicuous in the high-resolution X-ray spectrum of this object. I have explored the uncertainties in the irradiating spectral energy distribution due to the nuclear obscuration of the source and the effects these have on the survival of the dust, on the thermal stability of the warm absorber phases and the ionisation balance calculations required for photoionisation modelling.

From my case-studies of these three objects emerges a more detailed picture of the ionised outflows phenomenon and of the environment in the vicinity of the nuclear supermassive black holes in AGN.
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I dedicate this thesis to the memory of my beloved uncle and best friend, Majid (1967–2011), for all the happy times we spent together.
We have to remember that what we observe is not nature in itself but nature exposed to our method of questioning.

Werner Heisenberg
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Chapter 1

Introduction

The central region (nucleus) of an active galaxy is remarkably bright at all wavelengths. The enormous amount of radiation emitted from the nucleus is far more than can be produced by stars alone; the power is typically about $10^{36}$ to $10^{39}$ W. The widely accepted paradigm of the origin of energy in AGN is that they contain a central supermassive black hole (SMBH), with a typical mass of about $10^7$ to $10^9$ times that of the Sun ($M_\odot$), which is feeding on stars and gas in the galaxy. An accretion disc is formed around the black hole as matter flows in, releasing huge amounts of gravitational potential energy as radiation. The nucleus of an active galaxy is too small to be spatially resolved with current telescopes, so techniques such as spectroscopy and temporal variability analysis are used to probe into the structure of the nucleus and study the physical processes taking place in the vicinity of the SMBH.

The infall of matter is accompanied by outflows (winds of ionised gas and powerful collimated jets), which transport matter and energy away from the black hole. The absorption signatures of the ionised gas outflows are detected in the high-resolution UV and X-ray spectra of AGN. Understanding the structure, location and physical states of the outflows and their impact on their host galaxies is an active area of research. The soft X-ray outflows ("warm absorbers") consist of distinct phases of photoionised gas with temperatures of $10^4$–$10^6$ K, travelling at velocities of up to a few $10^3$ km s$^{-1}$. They are likely to be produced as the intense radiation released from the accretion disc blows off gas from a dusty gas torus thought to surround the SMBH and the accretion disc and in some cases obscure the direct emission. More highly ionised outflows, typically imprinting their signatures in
the hard X-ray band, travel at greater velocities ($\sim 10^4$ km s$^{-1}$) and are likely to originate in the form of winds from the accretion disc.

The continuous improvements in astronomical instrumentation at all wavelengths, in particular the breakthrough made by the advent of high-resolution X-ray spectrometers onboard XMM-Newton and Chandra, are providing new insights into the inflow and outflow processes in AGN. Yet, many aspects of these phenomena (such as the distribution of the energy budget between inflows, outflows and radiation for AGN systems of various scales and accretion rates) and their implications for the AGN environment are poorly understood. Outflows not only influence the immediate surroundings of the SMBHs at the cores of AGN, but also have far-reaching consequences. In AGN, the balance between accretion and outflows impacts the growth and evolution of SMBHs, star formation in their host galaxies, the surrounding intergalactic medium (IGM) and the cooling flows at the cores of clusters of galaxies to which they may belong. It is through this feedback that AGN shape the massive galaxy population, and this is now a standard paradigm in cosmological simulations of galaxy formation.

An illustration of the emitting (accretion disc, Broad and Narrow Line Regions) and absorbing structures (ionised absorber outflows) thought to be present in a Seyfert-type AGN (see Sect. 1.1) are shown in Fig. 1.1. These structures, their intrinsic optical/UV/X-ray emission, and the absorption by ionised outflows will be discussed in detail in Chapters 2 and 3. In this chapter, I will give an account of the history of AGN discoveries and observations (Sects. 1.1 and 1.2). The important developments in X-ray astronomy are traced, with the focus being on AGN. The unification scheme of AGN and their classification is described in Sect. 1.3. In Chapter 4, the XMM-Newton observatory, which has provided the vast majority of the data presented in this thesis, is described, as well as the data reduction. Chapters 5, 6 and 7 present the analysis and results obtained from the observations of the Seyfert galaxies NGC 3516, Mrk 509 and ESO 113-G010, respectively. Conclusions and implications are described in Chapter 8 and future work is proposed in Chapter 9.
Fig. 1.1: An illustration of the nested structures thought to be present in a Seyfert-type AGN.
1.1 History of optical and radio discoveries of AGN

The first observational evidence of an active galaxy was discovered by Edward A. Fath of Lick Observatory in 1908 as part of his dissertation work. A major question in the literature back then was whether spiral galaxies (or “spiral nebulae” as they were called at the time) were nearby gaseous nebulae (similar to planetary nebulae), or distant collections of unresolved stars. Fath undertook an investigation to test which scenario is correct. He constructed a spectrograph, designed for observing such “faint” spiral nebula sources, and mounted it on the 36-inch Crossley reflector telescope located at the Lick Observatory. He noted in his spectroscopic survey of the brightest spiral nebulae that almost all of them had a continuum spectrum with stellar absorption lines, which he correctly interpreted as the integrated light of a large number of stars. There was, however, one unusual object (NGC 1068), which had six emission lines in its spectrum; he identified them as the characteristic emission lines seen in planetary nebulae. This was the first time that the characteristic optical spectrum of an AGN was observed and noted. Fath’s findings were published in the Lick Observatory Bulletin (Fath 1909). Later on, the presence of emission lines in NGC 1068 was confirmed by others; in particular, Vesto M. Slipher of the Lowell Observatory obtained higher-quality spectra of NGC 1068 with resolved emission lines and reported line widths of hundreds of kilometres per second (Slipher 1917).

In the following years, the presence of emission lines in some other spiral nebulae was reported. In 1926, Edwin P. Hubble published his seminal paper on “extragalactic nebulae”, in which he classified them and also emphasised the presence of planetary-nebulae-type emission lines in some rare cases of spiral nebulae, notably, NGC 1068, NGC 4051 and NGC 4151 (Hubble 1926). The first systematic study of spiral galaxies with nuclear emission lines was published by Carl K. Seyfert in 1943. Seyfert realised that the majority of the spiral galaxies with emission features have low-ionisation emission lines, whereas only a small minority have high-ionisation lines. He then selected a sample of six of the brightest spiral galaxies with high-ionisation nuclear emission lines (NGC 1068, NGC 1275, NGC 3516, NGC 4051, NGC 4151 and NGC 7469) and made an intensive study of their spectra. He provided details of line strengths, line profiles and of the continuum (described by “colour temperatures”), and found that the emission lines of these objects are much
broader than the low-ionisation emission lines that occur in the spectra of many normal galaxies. Seyfert attributed the large widths of the lines to Doppler broadening, $\Delta \lambda / \lambda = \Delta v / c$, implying velocity ranges up to $\Delta v \sim 8500 \text{ km s}^{-1}$ (full width at zero intensity) for hydrogen lines of NGC 3516 and NGC 7469. These spectral properties of bright nuclei of spiral galaxies reported by Seyfert (1943) became the defining characteristics of the class of objects we call Seyfert galaxies today. Seyfert galaxies, however, received no further attention until after the optical identification of several of the strongest radio sources with galaxies.

The introduction of radio astronomy, coming from a different direction of research to optical astronomy, was crucial to the launch of AGN studies as a major focus of astronomical research. Karl G. Jansky, working at the Bell Telephone Laboratories, undertook a study of the sources of static affecting trans-Atlantic radio communications (Jansky 1932). His investigation lead to the discovery of radio emission from the disc of the Milky Way, with the strongest emission coming from the direction of the Galactic centre (Jansky 1933, 1935). Although Jansky’s work did not receive serious attention at the time, it eventually paved the way for scientists and radio engineers to focus on radio astronomy. Discrete radio sources, such as Cygnus A, were soon discovered (Reber 1944; Hey et al. 1946; Bolton and Stanley 1948a; Bolton 1948b; Ryle and Smith 1948).

The optical identification of discrete radio sources (other than the Sun) started with Bolton et al. (1949). They identified Taurus A with the Crab Nebula, Virgo A with M87 and Centaurus A with NGC 5128. In the 1950s, more progress was made in position determination and optical identification of radio sources. Importantly, Baade and Minkowski (1954) made the optical identification of Cygnus A with a galaxy. Its rich emission-line optical spectrum was found to show broadening of the high-ionisation lines, similar to the spectra of Seyfert galaxies. Thus, Cygnus A radio and optical characteristics became signatures on which to base the identification of other similar radio galaxies, leading to the early radio surveys of the sky such as the third Cambridge (3C) catalog of radio sources (Edge et al. 1959).

In addition to radio galaxies, other celestial radio sources appeared to be star-like, with no traces of a galaxy or nebula in their optical images and were named “quasi-stellar radio sources” (QSRSs), or “quasars” for short. Their optical spectra showed broad emission lines superimposed on the continuum and no absorption
lines. One of the first quasars to be discovered was 3C 48; at the American Astronomical Society meeting of 1960, Alan R. Sandage reported that optical photometry showed this object to be variable, with an excess UV emission compared with normal stars, and also that its optical spectrum displayed broad emission lines at unfamiliar wavelengths. No physically consistent interpretation was initially found for these peculiar radio sources. The general agreement at the time was that quasars are relatively nearby stars with very peculiar properties. The breakthrough came with the work of Maarten Schmidt on 3C 273 in 1963. From his spectral studies of this quasar, carried out with the 200-inch reflector telescope at the Palomar Observatory, he identified several well-known broad emission lines at what was then an unusually large redshift of \( z = 0.158 \) (Schmidt 1963). After this, redshifted emission lines in other quasars were identified; for example, Greenstein and Matthews (1963) identified several emission lines in 3C 48 at \( z = 0.367 \), making it one of the highest redshift galaxies known at the time.

One early suggestion for the origin of the redshift of quasar emission lines was gravitational redshift by very high density Galactic stars; however, this explanation was quickly discarded by Greenstein and Schmidt (1964) who argued the width of the lines required the line-emitting gas to be confined to a small fractional radius around the star; also the observed symmetry of the lines was inconsistent with a gravitational redshift scenario. Soon it became clear that quasars were highly luminous extragalactic objects, with redshifts reflecting Hubble’s expansion of the universe. High luminosity quasi-stellar objects without radio emission were also found; e.g. Sandage (1965) reported the discovery of a large population of such objects, which were named “radio-quiet” quasars (RQQs), or simply quasi-stellar objects (QSOs). Nowadays, the distinction between quasars and QSOs has somewhat faded and both classes are referred to as quasars by the research community. Quasars are so luminous and distant that the galaxies in which they reside could not be detected in early photographic images. The host galaxies of quasars were eventually resolved with charge-coupled device (CCDs) and improvements in imaging detectors, confirming that they are luminous AGN at high redshifts. Active galactic nuclei revolutionised astronomy in the 1960s as they pushed back the limits of the observable Universe; their compact size and enormous luminosities could not be explained in terms of what was known of stars and galaxies at the time, and as a
1.2 History of X-ray discoveries of AGN

Cosmic X-ray observations, requiring instruments to operate above the Earth’s absorbing atmosphere, had to wait for the beginning of the space age to become feasible. A group at American Science and Engineering (AS&E), led by Riccardo Giacconi, discovered the first extrasolar X-ray source. In June 1962, the AS&E Geiger counter instrument, originally intended to detect X-rays from the Moon, was successfully launched on an Aerobee 150 sounding-rocket. As it turned out, Giacconi et al. (1962) discovered the X-ray background and a powerful X-ray source in the constellation of Scorpius, known as Sco X-1. Apart from the Sun, Sco X-1 is the brightest source of X-rays in the sky, and as we know today, it is a low-mass X-ray binary system consisting of a neutron star accreting matter from a companion star. This discovery by Giacconi et al. (1962) captured the interest of the astronomical community and started the exploration of cosmic X-ray sources. During the years of sounding rocket experiments using proportional counters, the first X-ray identifications of AGN were made. Friedman and Byram (1967) reported detection of X-rays from M 87 and 3C 273; Bowyer et al. (1970) confirmed these two X-ray detections and also discovered X-rays from NGC 5128 (Centaurus A).

**Uhuru**, known before launch as the Small Astronomical Satellite 1 (SAS-1), was the first satellite dedicated to X-ray astronomy. It was equipped with two sets of proportional counters, each with an effective area of 840 cm$^2$, operating in the 2–20 keV energy range. It was launched on 12 December 1970 from the San Marco platform in Kenya; since it was launched on the anniversary of the independence of Kenya, the satellite was named Uhuru, which means “freedom” in Swahili. **Uhuru** operated until 1973 and performed the first comprehensive and uniform all sky X-ray survey with a sensitivity of $1.5 \times 10^{-11}$ erg cm$^{-2}$ s$^{-1}$ in the 2–20 keV range, or $5 \times 10^{-4}$ the flux from the Crab Nebula. One of the scientific highlights of the mission was the discovery of X-rays from two AGN, the Seyfert galaxies NGC 1275 and NGC 4151 (Gursky et al. 1971). Soon other missions followed which made significant contributions to X-ray astronomy, such as Orbiting Solar Observatory 7 (OSO-7, 1971), *Copernicus* (1972), *Ariel-V* (1974) and SAS-3 (1975).

During the 70s, X-ray variability of AGN was discovered, although detecting it
was made difficult by comparing results from different satellites. From OSO-7 observations, Winkler and White (1975) discovered an X-ray flux increase of a factor of at least 1.6 in Centaurus A over a period of 6 days. The first studies which established the power-law shape of the X-ray spectrum of a Seyfert galaxy were performed on NGC 4151 by Baity et al. (1975) and Ives et al. (1976), using proportional counter data from OSO-7 and Ariel-V satellites, respectively. Ives et al. (1976) also found a significant increase in the X-ray flux of NGC 4151 compared to earlier Uhuru observations. However, AGN were first understood to be generally strong X-ray emitters by Elvis et al. (1978) as a result of an Ariel-V survey. They identified 13 Seyfert galaxies, 11 of which had not been previously identified as X-ray emitters. The power radiated in the 2–10 keV band was reported to be typically in the range $10^{42.5} - 10^{44.5}$ erg s$^{-1}$, and to be correlated with the infrared and optical continuum powers, and with the luminosity in the H$\alpha$ emission line. The Elvis et al. (1978) results established powerful X-ray emission as a characteristic property of Seyfert galaxies. From Ariel-V observations over a period of 5 years, Marshall et al. (1981) found evidence for variability by a factor of up to 2 on timescales of less than a year in about half of the 28 AGN which they had investigated. X-ray flux variability on a timescale of 0.5–5 days was also reported for some of the AGN.

Beginning in 1977, NASA set the pace in X-ray astronomy by launching a series of large scientific missions called High Energy Astronomy Observatories (HEAO). The first of these missions, HEAO-1, surveyed the X-ray sky almost three times over the 0.2 keV–10 MeV energy band, and gathered data on a sufficient sample of objects to allow comparisons of different classes of AGN and monitor their variability. Using HEAO-1 observations, Singh et al. (1985) discovered that, apart from the X-ray power-law, there is another spectral component present in the spectrum of the bright Seyfert Mrk 509: the “soft X-ray excess”, which is an excess continuum emission above the extrapolated 2–10 keV power-law at the soft X-ray energies below 2 keV. HEAO-2 (the Einstein Observatory), again led by the Giacconi team, featuring grazing incidence focusing optics, marked another milestone in the advance of the X-ray astronomy, being the first fully imaging X-ray telescope. With an angular resolution of few arcsec, a field-of-view of tens of arcmin and a sensitivity several hundred times greater than any previous mission, it provided for the first time the capability to image extended objects and diffuse emission, and carry out surveys.
to detect sources as faint as $\sim 1.3 \times 10^{-14}$ erg cm$^{-2}$ s$^{-1}$ in the 1–3 keV band (Giacconi et al. [1979]). From *Einstein* data, QSOs were recognised as a class of X-ray emitters (Tananbaum et al. [1979]) and X-ray emission was established as a characteristic of all types of AGN and a valuable diagnostic of their innermost workings. Interestingly, the first X-ray warm absorber identification was also made using the *Einstein* data by Halpern ([1984]). Detection of X-ray jets from Centaurus A (Schreier et al. [1979]) and M87 (Lea et al. [1982]), aligned with the radio jets, were also AGN-related discoveries of the *Einstein* Observatory.

Following the end of the HEAO missions in 1981, there was a lengthy gap before the next X-ray astronomy mission was launched by NASA. Meanwhile, the progress of X-ray astronomy was taken forward by the launch of the European X-ray Observatory Satellite (EXOSAT) by the European Space Agency (ESA) in 1983 and the Japanese X-ray satellite *Ginga* in 1987. With its highly eccentric orbit and long (~ 4 days) uninterrupted observing capability, EXOSAT provided the means for a comprehensive study of AGN variability and thus rapid variability was also established to be common in AGN. Shortly after the discovery of the soft X-ray excess in Mrk 509 by Singh et al. ([1985]) using HEAO-1 data, the presence of a soft X-ray excess was also reported in the Seyfert galaxy Mrk 841 by Arnaud et al. ([1985]) using the combined low energy (0.02–2.5 keV) and medium energy (1.5–15 keV) response of the EXOSAT X-ray instruments. The EXOSAT data showed the soft X-ray excess emission component below 1 keV to be a common feature of the X-ray spectra of Seyfert galaxies. Spectral features near 7 keV, attributed to fluorescence and absorption of K-shell iron, were also discovered in several AGN spectra obtained by *Ginga* (Nandra and Pounds [1994]).

The German Roentgen Satellite (ROSAT) was launched in 1990, carrying a high-resolution X-ray imaging telescope that would undertake the first deep all-sky survey with imaging optics, cataloguing more than 150000 X-ray sources. ROSAT’s improved sensitivity and spectral resolution below ~ 2 keV showed further unexpected spectral features, indicating a surprisingly large column density of ionised gas (the “warm absorber”) in the line of sight to the nucleus of many Seyfert galaxies. The sequence of international X-ray astronomy missions continued, notably with the Japanese Advanced Satellite for Cosmology and Astrophysics (ASCA) launched in 1993, the US Rossi X-ray Timing Explorer (RXTE) launched in 1995 and the
Dutch-Italian *BeppoSAX* mission in 1996 (Space Science Department of ESA were also involved in the development of *BeppoSAX*). The improved spectral resolution of ASCA and timing capability of RXTE provided further scientific returns from X-ray studies of AGN.

The launch of *Chandra* and *XMM-Newton* observatories in 1999 opened a new era in X-ray astronomy and high energy astrophysics, providing unprecedented high spatial resolution with *Chandra* and unparalleled high-throughput spectroscopy with *XMM-Newton*. The exciting results and detailed studies emerging from these two still active missions have hugely advanced our knowledge of AGN physics, which is the subject of this thesis. *XMM-Newton* is the main X-ray observatory used for the studies presented in this thesis; thus in Sect. 1.3 the satellite and its scientific instruments are introduced and described.

### 1.3 Unification scheme and classification of AGN

The optical/UV and radio studies of AGN, together with the associated results obtained over the years by the X-ray astronomy missions described in the previous section, have led to the construction of a *Unified Model* of AGN. According to this, the range of observed properties of AGN is tentatively explained as due to different viewing angles of the observer. In this model, the central SMBH and the accretion disc are surrounded by an optically-thick torus of molecular gas and dust. The dusty torus, which is heated by the accretion disc radiation, reprocesses emission from the disc into mainly the infrared band. Within the torus, there are gas clouds which are heated by the radiation from the accretion disc; these clouds give rise to the broad optical/UV emission lines. There are also gas clouds further out from the torus, which still receive radiation from the accretion disc; these clouds give rise to narrow optical/UV emission lines. If the observer’s view is not obscured by the torus, then the central region is visible and thus emission lines from both the broad-line region (BLR) and narrow-line region (NLR) would be seen in the optical/UV spectra of the AGN. In this case, the AGN is called a Type-1 AGN. However, if the observer views the AGN through the dusty torus, then the BLR clouds are hidden and only the NLR clouds are visible; in this case only narrow emission lines are observed in the optical/UV spectra and the AGN is known as a Type-2. Therefore, we have the distinction between Seyfert-1 and Seyfert-2 galaxies, which are radio-
quiet Type-1 and Type-2 AGN, respectively. Similarly, *broad-line radio galaxies* (BLRGs) are radio-loud Type-1 AGN and *narrow-line radio galaxies* (NLRGs) are radio-loud Type-2 AGN.

In radio-loud AGN, we often observe high-speed jets of plasma being emitted from the nucleus, and travelling along what we assume to be the axis of the accretion disc; the jets are thought to be responsible for the synchrotron radio emission from the nucleus and the radio lobes at the end of the jets. The appearance of a radio-loud AGN also depends on the viewing angle. If the jet were viewed nearly end-on, the AGN would be classified as a *blazar*, which commonly shows superluminal motion indicating relativistic outflow velocities close to our line of sight. However, if viewed at other angles away from the jet axis towards the plane of the disc and the torus, then the radio-loud AGN is classified as a *radio galaxy*, with radio lobes on either side of the nucleus.

Blazars divide into two categories: *BL Lac objects* and *optically violently variable* (OVV) quasars, which were first recognised as distinct classes of objects from their observational characteristics by Strittmatter et al. (1972) and Penston and Cannon (1970), respectively. The characteristic feature of BL Lac objects is a featureless continuum spectrum with no emission or absorption lines, although weak stellar absorption features or weak nebular emission lines can be detected in very high signal-to-noise ratio spectra (e.g. Sbarufatti et al. 2006). OVV quasars, however, have strong optical/UV emission lines which resemble those of non-beamed AGN. Whilst in blazars we are looking down the relativistic jet, in radio galaxies with extended radio structures, the jet is projected onto the sky.

Radio galaxies are divided into two separate luminosity classes: Fanaroff and Riley (1974) Class I (FR I) and Class II (FR II). FR Is are weaker radio sources, with only a bright jet at the nucleus, with decreasing surface brightness towards the edge of the radio lobes. In contrast, in the more luminous FR IIs, the radio jet extends from the radio-faint nucleus to the extended powerful radio lobes which are brightest at the edges of the lobes. BLRGs and NLRGs are luminous FR II galaxies; in the context of the Unified Model, if FR II galaxies are observed along the axis of the jet, then they would be recognised as OVV quasars. On the other hand, if the less luminous FR I galaxies with their bright central radio jet were observed along the axis of the jet, they would be regarded as BL Lac objects (see
1.3. Unification scheme and classification of AGN

The QSOs, i.e. radio-quiet quasars (RQQs), are also Type-1 AGN and are thought to be the higher-luminosity version of Seyfert-1 galaxies, often at higher redshifts than Seyferts. However, it is not very clear which objects correspond to the higher-luminosity version of Seyfert-2 galaxies (i.e. the Type-2 QSOs). It has been debated that ultra-luminous infrared galaxies (ULIRGs) are such candidates (e.g. Tran et al. 2000), whose emission predominantly emerges in the far-IR via reprocessing of optical/UV/X-ray radiation by cold dust. Observations suggest that the obscuring dust is being heated by AGN, although the dust could also be heated by starbursts, i.e. large numbers of recently formed stars (see e.g. review of Sanders and Mirabel 1996). However, more recently, X-ray surveys have been crucial in finding the sought-after “classic” Type-2 QSOs, which, based on the Unified Model, are predicted to display narrow permitted emission lines, powerful hard X-ray emission, and a high equivalent width (EW) Fe Kα line (Ghisellini et al. 1994). For example, Norman et al. (2002) have discovered such a Type-2 QSO at a redshift of 3.7 in the Chandra Deep Field South survey (Giacconi et al. 2001).

1.3.1 Observational classification of Seyfert-1 galaxies

Seyfert galaxies are the main type of AGN investigated in this thesis. Seyfert-1 galaxies have broad Hα, HeI and HeII emission lines in their optical and UV spectra with typical $\Delta v_{\text{FWHM}} \approx 5000$ km s$^{-1}$, whilst the forbidden lines such as [OIII] are narrower, with typical $\Delta v_{\text{FWHM}} \approx 500$ km s$^{-1}$. On the other hand, in Seyfert-2 galaxies the permitted and forbidden lines have approximately the same width, typically $\Delta v_{\text{FWHM}} \approx 500$ km s$^{-1}$. Seyfert-1 galaxies are further subdivided on the basis of the appearance of the optical spectrum, as proposed by Osterbrock (1981). In Seyfert-1 galaxies, Hα lines consist of a broad component (from the BLR) on which a narrow component (from the NLR) is superimposed. The relative strengths of the broad and narrow components vary in Seyfert-1 galaxies. As the broad component of the Hα lines become weaker relative to the narrow component, the Seyfert type changes from 1.0 to 1.2 to 1.5. As outlined in Osterbrock and Ferland (2006), Seyfert-1 galaxies with intermediate-type Hα profiles in which both the broad and narrow components can easily be recognised are classified as Seyfert 1.5 galaxies. Those with strong narrow components and very weak but still visible broad components of Hα $\lambda 6563$ and Hβ $\lambda 4861$ are classified as Seyfert 1.8; and those in which
the very weak component is only seen in H\textalpha{} and not in H\beta{} are called Seyfert 1.9. Those Seyferts in which no broad component is detected at all are the Seyfert-2 galaxies (i.e. the Type-2 AGN with the edge-on orientation).

Furthermore, there is a subset of Seyfert galaxies known as narrow-line Seyfert-1 galaxies (NLSy1s) which show very intense and variable soft X-ray emission, with very steep soft X-ray spectra (e.g. Boller et al. 1996). They have narrow permitted optical emission lines (H\beta{} FWHM $< 2000$ km s$^{-1}$) and prominent optical Fe\textsc{ii} emission (e.g. Osterbrock and Pogge 1985). The steep soft X-ray spectrum indicates a higher accretion rate and a smaller black hole mass compared to the ‘normal’ broad-line Seyfert galaxies (e.g. Pounds et al. 1992).
Chapter 2

Emission from Seyfert type AGN

Over the last few decades broad-band studies of AGN emission and its variability have been essential in developing our understanding of the physical structure of emitting regions in the vicinity of the supermassive black hole. In particular, multi-wavelength (optical/UV/X-ray) monitoring of the AGN variability is a most effective way to investigate complex phenomena such as the accretion onto a SMBH, and provides diagnostics of the processes in the nuclear environment of AGN.

2.1 Optical/UV continuum from the accretion disc

The most prominent feature of AGN Spectral Energy Distributions (SEDs) is the so-called “big-blue-bump” peaking in the extreme UV, which was first attributed to thermal emission from the accretion disc by Shields (1978); this has since become the generally agreed paradigm. As a mass $m$ in the accretion disc moves inwards towards the black hole, gravitational potential energy is released. For an annulus of the disc lying between distance $r - dr$ and $r$ from a central black hole of mass $M$, gravitational potential energy is released at the rate $(GM\dot{M}/r^2) dr$, where $G$ is the gravitational constant and the mass accretion rate $\dot{M} = dm/dt$. From the virial theorem, half of the released potential energy is converted to kinetic energy (i.e. heating up of the gas) and the other half is radiated away at rate $dL$; therefore, $dL = (GM\dot{M}/2r^2) dr$. Assuming the energy is dissipated locally and the medium is optically thick, the local emission can be approximated by a blackbody, therefore, $dL = \sigma T^4 dA$, where $\sigma T^4$ is the power radiated per unit area $dA$ according to the Stefan-Boltzmann law. The area of the annulus $dA = 2(2\pi r) dr$, where the factor 2 takes into account radiation coming from both sides of the accretion disc.
2.1. Optical/UV continuum from the accretion disc

From rearranging the above expressions for $dL$, the local temperature at radius $r$ in the disc is $T = (GM\dot{M}/8\pi r^3\sigma)^{1/4}$. However, this does not take into account how the energy is dissipated in the disc, which is a consequence of work done by viscous torques (see e.g. Frank et al. 2002). Taking these into account, the radial temperature profile for a steady-state geometrically thin, optically thick Shakura-Sunyaev accretion disc (Shakura and Sunyaev 1973) is given by

$$T(r) = \left\{ \frac{3GM\dot{M}}{8\pi r^3\sigma} \left[ 1 - \left( \frac{R_{\text{in}}}{r} \right)^{1/2} \right] \right\}^{1/4} \quad \text{(2.1)}$$

where $R_{\text{in}}$ is the radius at the inner edge of the disc. Note that for $r \gg R_{\text{in}}$, $T(r) = T_*(r/R_{\text{in}})^{-3/4}$, where $T_* = (3GM\dot{M}/8\pi R_{\text{in}}^3\sigma)^{1/4}$. From Eq. (2.1) the maximum temperature in the disc, $T_{\text{max}}$, occurs at $r = (49/36)R_{\text{in}}$, thus $T_{\text{max}} \approx 0.488T_*$. The spectrum emitted by each element of area of the disc can be approximated using the Planck’s law as

$$I_\nu = B_\nu(T) = \frac{2h\nu^3}{c^2 \left( e^{h\nu/k_BT} - 1 \right)} \quad \text{(2.2)}$$

where $I_\nu$ is the spectral intensity in units of erg s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ sr$^{-1}$, $B_\nu(T)$ is the Planck function, $\nu$ the frequency, $h$ the Planck constant, $k_B$ the Boltzmann constant and $c$ the speed of light. Annuli of the disc at different radii have different temperatures and therefore the disc spectrum is the weighted sum of different blackbody spectra. The flux at frequency $\nu$ from the disc seen by an observer at distance $d$ whose line of sight makes an inclination angle $i$ to the normal of the disc plane is given by

$$F_\nu = \frac{2\pi \cos i}{d^2} \int_{R_{\text{in}}}^{R_{\text{out}}} I_\nu \, r \, dr \quad \text{(2.3)}$$

since a ring on the disc between $r$ and $r + dr$ subtends a solid angle $2\pi \cos i \, r \, dr / d^2$; $R_{\text{out}}$ is the radius at the outer edge of the disc. Substituting Eq. (2.2) into Eq. (2.3) gives

$$F_\nu = \frac{4\pi h\nu^3 \cos i}{c^2 d^2} \int_{R_{\text{in}}}^{R_{\text{out}}} \frac{r}{e^{h\nu/k_BT(r)} - 1} \, dr \quad \text{(2.4)}$$

The shape of the emitted spectrum can be deduced for different frequency regimes. In the low-frequency regime, $h\nu \ll k_BT_{\text{out}}$, the Planck function takes the Rayleigh–Jeans form $B_\nu(T) = 2k_BT\nu^2/c^2$, hence $F_\nu \propto \nu^2$. In the high-frequency regime, $h\nu \gg k_BT_*$, the Planck function follows the Wien law $B_\nu(T) = 2h\nu^3 e^{-h\nu/k_BT} / c^2$, hence $F_\nu \propto \nu^3 e^{-h\nu/k_BT_*}$ and the spectrum is dominated by
the hottest regions of the disc \((T \sim T_*)\) with an exponential cut-off. In the intermediate-frequency regime, \(k_B T_{\text{out}} \ll h\nu \ll k_B T_*\), Eq. (2.1) can be approximated as \(T(r) \approx T_*(R_{\text{in}}/r)^{3/4}\); substituting \(x = h\nu/k_B T(r) \approx (h\nu/k_B T_*)(r/R_{\text{in}})^{3/4}\) into Eq. (2.4) gives \(F_\nu \propto \nu^{1/3}\). Thus, in the intermediate frequency regime, where most of the energy is emitted, the spectrum is flatter with \(F_\nu \propto \nu^{1/3}\); this is a characteristic of the accretion disc spectrum which appears like a stretched-out blackbody spectrum, as shown in Fig. 2.1.

An important feature of the predicted emitted spectrum of Eq. (2.4) is its independence from the unknown disc viscosity. This is a consequence of both the steady-state thin disc and blackbody assumptions. If these assumptions are valid for the accretion disc of AGN, one expects the spectrum specified by Eq. (2.4) to give a fairly good representation of the observed spectrum (i.e. the big-blue-bump in AGN). Indeed, the observed big-blue-bump is usually successfully fitted with such an underlying disc blackbody model. Figure 2.1 shows an example of a disc blackbody spectrum \(F_\nu\) fitted to the optical/UV continuum data of Mrk 509 (see Sect. 6.4.2) using the \texttt{dbb} model in the \textsc{spex}† spectral fitting package (Kaastra et al. 1996), which is the same disc model described above. The parameter \(R_{\text{out}}\) cannot be constrained by spectral fitting since most of the optical/UV radiation originates from the inner regions of the disc for a SMBH, where the temperature is higher, thus \(R_{\text{out}}\) is fixed to \(10^3 R_{\text{in}}\). The fitted parameters of the model are the normalisation area \(A = R_{\text{in}}^2 \cos i\) and the maximum temperature of the disc \(T_{\text{max}}\). For the example shown in Fig. 2.1, \(A = 6.7 \times 10^{28}\) cm\(^2\) and \(T_{\text{max}} = 3.9\) eV, which has provided a good fit to the data.

### 2.2 Emission from the BLR and NLR

#### 2.2.1 The BLR

The characteristic emission from the BLR in a Seyfert-1 galaxy includes broad optical lines, such as the H\(\alpha\) \(\lambda6563\), H\(\beta\) \(\lambda4861\), H\(\gamma\) \(\lambda4340\) and H\(\delta\) \(\lambda4101\) Balmer lines, He\(\text{I}\) \(\lambda5876\) and He\(\text{II}\) \(\lambda4686\); and broad UV lines, such as Ly\(\alpha\) \(\lambda1216\), C\(\text{IV}\) \(\lambda1549\), C\(\text{III}\) \(\lambda1909\) and Mg\(\text{II}\) \(\lambda\lambda2796, 2803\). Furthermore, between \(\sim 2000\) and \(4000\) Å, an emission feature known as the “small-blue-bump” is observed, which consists of blended Fe\(\text{II}\) emission lines and Balmer continuum emission (Wills et al. 1983).

† http://www.sron.nl/spex
2.2. Emission from the BLR and NLR

Fig. 2.1: The continuum spectrum $F_{\nu}$ (Eq. 2.4) of a steady geometrically thin, optically thick accretion disc radiating locally as a blackbody, with $T_{\text{max}} = 3.9$ eV, area $A = 6.7 \times 10^{28}$ cm$^2$ and $R_{\text{out}} = 10^3 R_{\text{in}}$. This disc spectrum is from a spex dbb model fit to the optical/UV data of Mrk 509 (see Sect. 6.4.2) which are shown in red, plotted in the observed frame.

All the BLR lines are permitted or intercombination (semi-forbidden) lines, with no forbidden lines having such broad profiles. The only known interpretation for this is that the electron density $n_e$ of the BLR is so high (i.e. above a critical density $n_c$) that all the levels of the ions which could give rise to forbidden-line transitions are collisionally de-excited. The forbidden lines are weakened by a factor of $n_c/n_e$ from the strengths they would have with respect to the permitted lines (e.g. H$\beta$), at the same temperature and ionisation but in the low-density limit. In well-observed AGN, any possible broad component of the forbidden line [O III] $\lambda$5007 ($^1D_2$ to $^3P_2$ level transition) is found to be at most 1% the strength of H$\beta$ (Osterbrock and Ferland 2006). Since the critical density $n_c$ for O III ions in level $^1D_2$ is about $10^6$ cm$^{-3}$ (Osterbrock and Ferland 2006), a rough lower limit to the mean electron density in the BLR is $n_e > 10^8$ cm$^{-3}$. Furthermore, the critical density for collisional de-excitation of O III in level $^1S_0$ (the upper level for the
2.2. Emission from the BLR and NLR

The [O III] $\lambda 4363$ transition) is about $10^8 \text{ cm}^{-3}$ (Peterson 1997). Since this forbidden line is observed to have no broad component, this provides a similar lower limit estimate for the electron density $n_e > 10^8 \text{ cm}^{-3}$ in the BLR.

The semi-forbidden C III] $\lambda 1909$ line can be used to set a rough upper limit to the density in the BLR. This line is the only non-permitted line, observed in spectra of many AGN, to display a strong broad profile similar to H I profiles (see e.g. Peterson 1997). The critical density for de-excitation of the $^3P_1$ level in the C III ion from which this line arises is about $10^{10} \text{ cm}^{-3}$ (Osterbrock and Ferland 2006). Thus, the upper-limit for electron density in the C III] line-emitting zone of the BLR is roughly $10^{10} \text{ cm}^{-3}$.

The observed width (FWHM) of the broad emission lines, $\Delta v \lesssim 10000 \text{ km s}^{-1}$, and maximum wing widths of up to $30000 \text{ km s}^{-1}$, can only be interpreted as Doppler broadening. Such broad widths cannot be due to thermal broadening; the temperature of a gas in such thermal motion would be $k_B T \sim m_p (\Delta v)^2/2 \sim 1 \text{ MeV}$, i.e. $T \sim 10^{10} \text{ K}$. At this high temperature the observed emission lines cannot be produced since the atoms would be fully ionised; also in such high energy plasmas electron-positron annihilation ($e^- + e^+ \rightarrow \gamma + \gamma$) would come into play producing the corresponding 511 keV gamma-ray line (which is not observed). Furthermore, the observed Fe II emission indicates that $T < 35000 \text{ K}$, otherwise iron would be nearly completely ionised to Fe III, even if there were no ionising photons present (Osterbrock and Ferland 2006). The ionisation stages of the line-emitting elements and photoionisation modelling of the BLR rather indicate temperatures of the order of $10^4 \text{ K}$.

The width of the BLR lines can be attributed to Doppler broadening caused by large-scale motions with velocities of the order of 10000 km s$^{-1}$ in the presence of a strong gravitational field, as would occur in the vicinity of a SMBH. Assuming rotational motion for the BLR around the black hole and a simple virial argument, $v_{\text{rot}} \sim (GM_{\text{BH}}/r)^{1/2}$, so the radial distance $r$ from the black hole can be estimated. Using the Schwarzschild radius $R_S = 2GM_{\text{BH}}/c^2$ (corresponding to the event horizon for a non-rotating black hole), $r = R_S c^2/2v_{\text{rot}}^2$. For a BLR rotational velocity of 10000 km s$^{-1}$, $r \sim 450 R_S$; so, for a $10^8 \text{ M}_\odot$ black hole, the BLR is at a radial distance of about 0.0043 pc or 5 light days.

Emission line fluxes vary with time in a way that is highly correlated with the
AGN intrinsic continuum flux (e.g. Peterson 1993), confirming a connection between the BLR and the continuum emission. This provides a convincing argument that BLR line emission is caused by photoionisation by the central source continuum emission. Observations show that the BLR emission responds to a change in continuum flux after a delay time $\Delta t$, which is due to light travel-time effects across the BLR, i.e. $\Delta t \sim r/c$. Thus, the BLR “reverberates” in response to continuum variations. From measurements of time delays (or ‘lags’) between the continuum and line-emission variations, the size of the BLR and also the mass of the black hole can be obtained. This technique, known as reverberation mapping, has been successfully applied to a few dozens of AGN. The measured time lags in different AGN are in the range of a few days to 100 days. Different emission lines respond with different time lags, with usually higher-ionisation lines responding faster than lower-ionisation lines. This indicates that the BLR has a radially stratified ionisation structure and maximum variability response of different lines occurs at different radii. For example, as shown in Peterson (1997), in the Seyfert 1.5 galaxy NGC 5548 the higher-ionisation lines such as He$\text{II} \lambda 1640$ and N$\text{V} \lambda 1240$ respond to continuum variations faster ($\Delta t \sim 2$ days) than lower-ionisation lines such as Ly$\alpha \lambda 1216$ ($\Delta t \sim 10$ days), the H$\alpha \lambda 6563$ and H$\beta \lambda 4861$ Balmer lines ($\Delta t \sim 17$ and 20 days, respectively) and the semi-forbidden C$\text{III]} \lambda 1909$ line ($\Delta t \sim 22$ days).

The nature and origin of the BLR is not well-understood and different scenarios have been proposed. The BLR is believed to be composite; photoionisation modelling of the BLR suggests that it is composed of a two-phase medium, in which cool ($T \sim 10^4$ K) BLR clouds are embedded (confined) in a lower-density hot ($T \sim 10^8$ K) intercloud medium (see e.g. Krolik et al. 1981; Blandford et al. 1990). In this scenario, the BLR clouds are thought to be in pressure equilibrium with the hot intercloud medium. Magnetic confinement is another mechanism to confine the BLR clouds (e.g. Rees 1987). There are also disc wind models proposed for the origin of the BLR clouds, such as continuum radiation pressure driven winds (e.g. Mathews 1986) and hydromagnetically driven winds (e.g. Emmering et al. 1992).

### 2.2.2 The NLR

In spectra of AGN, the narrow forbidden and permitted lines originate in the NLR, which is well outside the BLR. Whereas the size and structure of the BLR must be inferred indirectly by processes such as reverberation mapping, the NLR is suf-
ficiently extended that, in the nearby AGN, it can be spatially resolved with the HST, and even ground-based telescopes can resolve the outer parts of the NLR in some nearby AGN. The HST has provided some detailed images and spectra of the NLR, spanning a few tens of pc to a few kpc in size. The morphology of the NLR is different from that of the BLR; the NLR is confined to ionisation cones that emanate from the nucleus (see the example of NGC 5728 shown in Fig. 2.2). These cones are thought to be the result of anisotropy in the AGN, introduced on much smaller scales by the obscuring torus that surrounds the central source; thus the cones are probably perpendicular to the accretion disc. The NLR is typically approximately axisymmetric; the emission region can extend out to considerable distances, ~ 15–20 kpc, turning into the extended narrow-line region (ENLR), in contrast to the higher surface-brightness, higher-ionisation gas closer to the nucleus (i.e. the NLR).

Unlike in the BLR, the presence of forbidden lines indicates that the electron densities in the NLR are low enough that the forbidden transitions are not collisionally suppressed. At lower densities the physics of line production in the NLR is less complex than in the BLR; line ratios can be used to estimate physical properties of the ionised gas. The electron density \( n_e \) and electron temperature \( T_e \) are determined by measuring the intensity ratio of lines from a single ion (see e.g. Sect. 3.2.2). Line ratios from a single ion are used in order to avoid complications due to unknown abundances and ionisation fractions of the ions.

Well-known examples for density measurements are the ratios of the line fluxes \( F \) of \([\text{S} \, II] \ F(\lambda 6717)/F(\lambda 6731) \) and \([\text{O} \, II] \ F(\lambda 3726)/F(\lambda 3729) \) which in each case represent \( ^4S_{3/2} \rightarrow ^2D_{5/2} \) and \( ^4S_{3/2} \rightarrow ^2D_{3/2} \) transitions (Osterbrock and Ferland 2006). However, only \([\text{S} \, II] \) is used since the \([\text{O} \, II] \) lines are so close together to be heavily blended by Doppler broadening. Studies show that the line ratios yield electron densities \( n_e \sim 10^3 \text{–} 10^4 \text{ cm}^{-3} \). For measurements of the electron temperature \( T_e \), \([\text{O} \, III] \ \lambda \lambda 4363, 4959, 5007 \) and \([\text{N} \, II] \ \lambda \lambda 5755, 6548, 6583 \) lines can be used. These lines are suitable because they have very different excitation potentials, so that the rate at which the different levels are populated by collisions is highly temperature dependent. However, usually only \([\text{O} \, III] \) flux ratio is used as the \([\text{N} \, II] \ \lambda 5755 \) line is rather weak. The \([\text{O} \, III] \ F(\lambda 4959 + \lambda 5007)/F(\lambda 4363) \) is very sensitive to the relative collisional excitation rates of the \(^1S_0 \) and \(^1D_2 \) levels and thus has a strong
2.3 Intrinsic X-ray emission

Temperature dependence. The measurements yield $T_e \sim 1-2 \times 10^4$ K in the NLR (Osterbrock and Ferland 2006).

2.3 Intrinsic X-ray emission

The thermal accretion disc model described in Sect. 2.1 explains only the optical/UV continuum emission of the AGN (the big-blue-bump); thus, another mechanism is required to explain the prominent higher-energy emission of the AGN. It is plausible to assume the presence of an additional medium which emits the high-energy radiation. It is generally believed this additional medium is a hot corona of energetic electrons in the vicinity of the accretion disc, which up-scatters the lower-energy optical/UV photons from the disc to the X-ray band. This process (inverse Comptonisation) also explains the observed power-law shape of the X-ray continuum in AGN, as described in the next section.
2.3. Intrinsic X-ray emission

2.3.1 Inverse Comptonisation in a hot plasma

The energy-momentum conservation for scattering can be written as

\[ P_i + Q_i = P_f + Q_f \]  \hspace{1cm} (2.5)

where \( P_i \) and \( P_f \) are the initial and final 4-momenta of the photon, and \( Q_i \) and \( Q_f \) are the initial and final 4-momenta of the electron. The 4-momenta are \( P_i = (E_i/c) (1, n_i) \), \( P_f = (E_f/c) (1, n_f) \), \( Q_i = \gamma_i m (c, v_i) \) and \( Q_f = \gamma_f m (c, v_f) \), where \( E_i \) and \( E_f \) are the initial and final energies of the photon, \( n_i \) and \( n_f \) the initial and final directional unit vectors of the photon, \( v_i \) and \( v_f \) the initial and final 3-velocities of the electron, \( \gamma_i \) and \( \gamma_f \) the initial and final Lorentz factors of the electron, \( m \) mass of the electron and \( c \) the speed of light. Using Eq. (2.5) and the Lorentz invariants \( P_\mu P^\mu = 0 \) and \( Q_\mu Q^\mu = -m^2 c^2 \), one can eliminate \( Q_f \) to show that

\[ P_f \cdot P_i + P_f \cdot Q_i = P_i \cdot Q_i \]  \hspace{1cm} (2.6)

In three-vector notation, Eq. (2.6) can be written as

\[ \frac{E_i E_f}{c^2} (n_i \cdot n_f - 1) + \frac{E_f \gamma_i m}{c} (n_f \cdot v_i - c) = \frac{E_i \gamma_i m}{c} (n_i \cdot v_i - c) \]  \hspace{1cm} (2.7)

Introducing the scattering angle \( \theta \) (angle between incident and scattered photon) as \( n_i \cdot n_f = \cos \theta \) and auxiliary angles \( \alpha_i \) (angle between incident photon and incident electron) and \( \alpha_f \) (angle between scattered photon and incident electron) as \( n_i \cdot v_i = v_i \cos \alpha_i \) and \( n_f \cdot v_i = v_i \cos \alpha_f \), where \( v_i \) is the velocity of the incoming electron in \( \gamma_i = (1 - v_i^2/c^2)^{-1/2} = (1 - \beta_i^2)^{-1/2} \), and using Eq. (2.7), the final energy of the photon \( E_f \) after scattering is

\[ E_f = \frac{(1 - \beta_i \cos \alpha_i) E_i}{1 - \beta_i \cos \alpha_f + (E_i / \gamma_i mc^2)(1 - \cos \theta)} \]  \hspace{1cm} (2.8)

Using Eq. (2.8), one can see that if a low-energy photon \( (E_i \ll mc^2) \) is scattered by an electron at rest \( (v_i = 0) \), the result is \( E_f = E_i \) and so the scattering is elastic (i.e. the Thomson scattering). If the photon energy \( E_i \) is non-negligible in comparison with the energy \( mc^2 \) of the electron at rest, \( E_f < E_i \) and so we have inelastic scattering of photons, with transfer of photon energy to electrons (i.e. the Compton scattering). However, if the electron is moving \( (v \) non-zero), \( E_f > E_i \) and so the inelastic scattering causes transfer of electron energy to photons (i.e. the inverse Compton scattering).
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The angle $\alpha_i$ is random but $\alpha_f$ is strongly beamed in the direction of the velocity $\mathbf{v}_i$ of the electron for the case of relativistic electrons ($\beta_i \rightarrow 1$ and $\gamma_i \gg 1$), so one can approximate $\cos \alpha_f \approx 1$; taking $E_i \ll \gamma mc^2$, Eq. (2.8) gives $E_f \approx E_i (1 - \beta_i \cos \alpha_i) / (1 - \beta_i)$. As an example for a single scattering, taking $E_i = 4$ eV (energy of a typical UV photon), $E_f = 1$ keV (energy of a typical X-ray photon) and $\cos \alpha_i = 0$ (averaged over the angle), the electron is required to have $\beta_i \approx 0.996$ (i.e. $\gamma_i \approx 11.2$). However, in reality, a photon undergoes a multiple number of scatterings before it escapes the corona and so it can be up-scattered to high energies for the case of non-relativistic electrons.

In a thermal distribution of electrons, the typical velocity of an electron is given by $m \langle v^2 \rangle / 2 \approx 3 k_B T_e / 2$, thus, $\beta_i^2 \approx 3 k_B T_e / mc^2$. For non-relativistic scattering of photons by a thermal distribution of electrons with temperature $T_e$, the mean energy change in the photon energy is given by

$$\frac{\Delta E}{E_i} = \frac{4 k_B T_e - E_i}{mc^2}$$

(2.9)

where $\Delta E = E_f - E_i$. When $E_i \ll k_B T_e$, the photon gains energy due to the Doppler effect and so $\Delta E / E_i = 4 k_B T_e / mc^2$; in the opposite case, if $E_i \gg k_B T_e$, the photon loses energy due to the recoil effect. Thus the photons gain or lose energy in a random walk around the plasma cloud. The photon energy gain due to the Doppler effect along a random trajectory with time duration $t$ is determined by the Comptonisation parameter

$$y \equiv \frac{k_B T_e}{mc^2} N = \frac{k_B T_e}{mc^2} c \sigma_T n_e t$$

(2.10)

where $N = c \sigma_T n_e t$ is the average number of scatterings which photons suffer during random walking and $\sigma_T$ is the Thomson cross-section. If the plasma region has a length $l$, then the optical depth for scattering is $\tau = n_e \sigma_T l$ and the scattering probability is $e^{-\tau}$. From a random-walk argument, the number of scatterings $N \approx \max(\tau, \tau^2)$ [Rybicki and Lightman 1979]; thus the Comptonisation parameter $y$, given in Eq. (2.10) depends only on the electron temperature $T_e$ and the optical depth $\tau$.

The time evolution of a given initial radiation spectrum, due to Comptonisation in a plasma cloud of a given geometry needs to be solved to obtain the emerging
spectrum at time $t$ after multiple scatterings. To do this, Sunyaev and Titarchuk (1980) solved the Kompaneets equation

$$\frac{\partial n}{\partial y} = \frac{1}{x^2} \frac{\partial}{\partial x} x^4 \left( n + n^2 + \frac{\partial n}{\partial x} \right)$$

which describes the theory of Compton interaction of radiation with matter in the non-relativistic regime ($h\nu \ll mc^2$, $k_B T_e \ll mc^2$), where, $n$ is the photon number density, $x \equiv h\nu/k_B T_e$ is the dimensionless frequency and $y$ is the Comptonisation parameter, dependent on time $t$. The Soviet physicist A. S. Kompaneets published the derivation of this equation in 1956; in fact the equation had been derived in the late 1940s by him and others under the leadership of Y. B. Zeldovich, as part of the Soviet nuclear weapons programme. The derivation of the Kompaneets equation is non-trivial; Rybicki and Lightman (1979) give an outline of the derivation. The solution found by Sunyaev and Titarchuk (1980) for the flux density $F_\nu$ as a function of $x$ is

$$F_\nu(x) \propto \begin{cases} x^{\alpha+3} & \text{for } x \ll x_0 \\ x^{-\alpha} & \text{for } x_0 \ll x \ll 1 \\ x^3 e^{-x} & \text{for } x \gg 1 \end{cases}$$

where the spectral index $\alpha$ is

$$\alpha = \sqrt{9 + \frac{1}{y} - \frac{3}{2}}$$

and the dimensionless parameter $x_0 = h\nu_0/k_B T_e$, with $h\nu_0$ being the energy of the seed photons. Eqs. (2.12a) and (2.12b) show that for $x \ll x_0$ and $x_0 \ll x \ll 1$ (when recoil plays a negligible role compared to the Doppler effect), the emergent spectrum is a power-law. Note that the spectral index $\alpha$ depends only on the electron temperature $T_e$ and the optical depth $\tau$ of the plasma cloud. At high frequencies, $h\nu \gg k_B T_e$ (i.e. $x \gg 1$), recoil dominates, and Eq. (2.12c) shows that a Wien spectrum is formed.

The COMT model of SPEX that has been used in this work (see Sect. 6.5) is based on the Comptonisation model of Titarchuk (1994), with improved approximations for the parameter $\beta(\tau)$ which characterises the photon distribution over the number of scatterings which the soft photons undergo before escaping the plasma; for more details see the SPEX manual (Kaastra et al. 2012a). The seed photons in this SPEX component have a Wien law spectrum. The up-scattering Comptonising plasma
2.3. Intrinsic X-ray emission

Fig. 2.3: Top panel: the Comptonisation model spectrum computed by the COMT model in SPEX for $T_{\text{seed}} = 2$ eV, $T_e = 0.22$ keV and $\tau = 16.2$. Bottom panel: the COMT model spectrum for $T_{\text{seed}} = 2$ eV, $T_e = 8.3$ keV and $\tau = 3.0$. The model examples are based on fits to the Mrk 509 broad-band data (Sect. 6.5), used for modelling the soft X-ray excess (top panel) and the X-ray power-law (bottom panel).
is chosen to have a disc geometry; its parameters are the temperature $T_e$ and the optical depth $\tau$. The COMT component assumes spherical symmetry for the flux calculation. Figure 2.3 shows two examples of COMT model inverse Comptonisation of low-frequency photons ($T_{\text{seed}} = 2$ eV) in a warm corona with $T_e = 0.22$ keV and optical depth $\tau = 16.2$ (top panel) and in a hot corona with $T_e = 8.3$ keV and $\tau = 3.0$ (bottom panel). The two examples are based on fits to the Mrk 509 broad-band data (Sect. 6.5), and were used for modelling the soft X-ray excess (top panel) and the X-ray power-law (bottom panel).

### 2.3.2 X-ray reflection

In Sect. 2.3.1, the formation mechanism of the X-ray spectrum of an AGN via inverse Compton up-scattering of soft photons by electrons in a corona was described. In many astrophysical environments, X-rays will then interact with gas that is neutral or partially ionised, which causes other radiative mechanisms to come into play and have an impact on the emergent spectrum. In AGN, the produced power-law spectrum, as well as coming directly to us, also irradiates the accretion disc. The irradiation of the accretion disc, or any other gas, produces back-scattered radiation in our line of sight which is commonly known as the reflection spectrum. Following Basko et al. (1974), who first introduced X-ray reflection in X-ray astronomy in a study of the expected reflection from the normal star in a Galactic X-ray binary system, the total cross-section (due to absorption and scattering) for X-rays of frequency $\nu$ to first approximation is

$$\sigma(\nu) = \sigma_T + \sigma_{\text{ph}}(\nu)$$

(2.14)

where $\sigma_T$ is the Thomson cross-section and $\sigma_{\text{ph}}$ the photoionisation cross-section as a function of $\nu$ (see Sect. 3.1). Since $\sigma_{\text{ph}}(\nu) \propto \nu^{-3}$ (Eq. 3.1), Eq. (2.14) is approximated by

$$\sigma(\nu) = \sigma_T \left[ 1 + \left(\frac{\nu_0}{\nu}\right)^3 \right]$$

(2.15)

where, at $\nu > \nu_0$, the scattering cross-section $\sigma_T$ exceeds the photoionisation cross-section $\sigma_{\text{ph}}$. The single scattering albedo (i.e. ratio of scattering cross-section to the total cross section) is thus

$$\lambda(\nu) = \frac{\sigma_T}{\sigma(\nu)} = \left[ 1 + \left(\frac{\nu_0}{\nu}\right)^3 \right]^{-1}$$

(2.16)
2.3. Intrinsic X-ray emission

So the reflection probability is determined by the competition between electron scattering versus photoelectric absorption. At energies below \( h\nu_0 \), the photoelectric absorption dominates, and at energies above \( h\nu_0 \) the scattering dominates. The energy \( h\nu_0 \), at which \( \sigma_{ph} \approx \sigma_T \), is about 10 keV for solar abundances (see e.g. Morrison and McCammon 1983). Therefore, above 10 keV scattering dominates, leading to reflection. However, at higher energies the recoil effect becomes increasingly important; at every Compton down-scattering, some of the photon energy is transferred to the electron and so high energy photons lose a considerable part of their energy; this also leads to the probability of photoelectric absorption (which increases with decreased photon energy) increasing after each scattering. So the combination of photoelectric absorption of lower-energy photons on one hand, and Compton down-scattering of higher-energy photons on the other, gives rise to a broad characteristic hump in the reflected continuum peaking at around 20–40 keV, known as the Compton hump.

Following photoelectric absorption of an X-ray photon and ejection of a K-shell electron of an atom, the excited ion de-excites by filling the K-shell hole with an outer electron. The released energy emerges either as an Auger electron or a K-shell fluorescent emission line. The K-shell fluorescence yield \( Y_K \) is an increasing function of the atomic number \( Z \) (\( Y_K \propto Z^4 \)), and so the element with the highest product of \( Y_K \) and abundance is iron (see Bambynek et al. 1972 and George and Fabian 1991). Thus, the fluorescence line emission is particularly strong for iron. The Fe K\( \alpha \) line, consisting of two components at energies 6.404 keV and 6.391 keV and relative intensities 2:1, makes the largest contribution to the fluorescent emission of neutral iron (Bambynek et al. 1972). Furthermore, the low atomic number elements are more likely to de-excite via Auger ionisation (ejection of an outer electron) rather than fluorescence emission.

Cold reflection (described above) refers to reflection from neutral material (in which the metals exist as atoms); in this case the reflection spectrum forms a small contribution to the total spectrum below a few keV compared to the incident X-ray continuum and so is too weak to be seen against the dominant X-ray power-law. Figure 2.4, based on Monte-Carlo calculations by George and Fabian (1991), shows an example of the cold reflection spectrum including X-ray fluorescence emission. The Compton hump at around 20 keV, fluorescence emission lines (notably the Fe
2.3. Intrinsic X-ray emission

Fig. 2.4: Example of a cold X-ray reflection model spectrum, produced when an X-ray power-law continuum with energy index $\alpha = 0.7$ (i.e. photon index $\Gamma = 1.7$) irradiates a slab of cold matter with cosmic abundances. The Compton hump at around 20 keV, fluorescence emission lines (notably the Fe K$\alpha$ line) and the Fe K-edge at around 7.11 keV appear prominently. The calculated spectrum is based on the Georg e and Fabian (1991) model. Figure taken from Peterson (1997).

Fig. 2.5: Examples of ionised X-ray reflection model spectra, produced when a X-ray power-law continuum with $\Gamma = 2.0$ irradiates a slab of ionised matter with cosmic abundances, for three different ionisation parameters $\xi$ (see Sect. 3.1). Figure taken from Ross and Fabian (2005).
2.3. Intrinsic X-ray emission

Kα line) and the Fe K-edge at around 7.11 keV appear prominently. However, ionised reflection (i.e. reflection from ionised material) is sensitive to the ionisation state of the reflecting material. The absorption cross-section changes as a function of the ionisation state, with opacity at low energies decreasing as the ionisation state increases, thus causing an increase in reflection at low energies. The ionised reflected spectrum at lower-energies contains other emission lines and recombination continua (see Sect. 3.2.3), which require more detailed modelling than cold reflection. Figure 2.5 taken from Ross and Fabian (2005), shows ionised reflection from a slab at different ionisation parameters (see Sect. 3.1, Eq. 3.8), leading to an increased reflection spectrum at larger ionisation parameters.

Since the start of X-ray reflection modelling by Lightman and White (1988), there has been a lot of interest and development in X-ray reflection computations, with several models being available in the xspec† spectral fitting package (Arnaud 1996). George and Fabian (1991) studied cold reflection with Monte-Carlo computations of X-ray fluorescent emission; Matt et al. (1991) calculated spectral characteristics produced by cold reflection such as line intensities and angular dependencies. Using a Monte Carlo method, Magdziarz and Zdziarski (1995) derived approximations to Green’s functions for Compton reflection, available as the pexrav and pexriv models in xspec; these are used for modelling reflection of an exponentially cut-off power-law spectrum from neutral (pexrav) and ionised (pexriv) material. More recent models of ionised reflection in xspec include the reflionx of Ross and Fabian (2005) and rfxconv described in Kolehmainen et al. (2011).

2.3.3 The soft X-ray excess

Apart from the power-law, the X-ray continuum of AGN often comprises another component, the “soft X-ray excess” i.e. a steepening of the spectrum at low energies, above an extrapolation of the X-ray power-law. Since its discovery in 1985, a soft excess has been observed in the X-ray spectra of the majority of AGN and understanding its origin remains an area of active research to this date. Different interpretations for the nature of the soft X-ray excess can be found in the literature such as: (1) the high energy tail of the thermal emission from the accretion disc (e.g. Arnaud et al. 1985, Pounds et al. 1986); (2) an artefact of strong, relativistically smeared, partially ionized absorption in a wind from the inner disc (e.g.

† http://heasarc.gsfc.nasa.gov/xanadu/xspec
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Gierliński and Done (2004); (3) part of the relativistically blurred photoionised disc reflection spectrum modelled by Ross and Fabian (2005) (e.g. Crummy et al. 2006); (4) ‘warm’ Comptonisation: up-scattering of seed disc photons in a Comptonising medium which has lower temperature and higher optical depth than the corona responsible for the X-ray power-law emission (e.g. the study by Magdziarz et al. 1998 of the Seyfert-1 NGC 5548; the analyses by Middleton et al. 2009 and Jin et al. 2009 of two NLSy1s: RE J1034+396 and RX J0136.9-3510). Chapter 6 reports the results of an unprecedented long multi-wavelength campaign on Seyfert-1 galaxy Mrk 509 which have established the origin of the soft excess in this object to be warm Comptonisation, based on the variability of the emission components.
Chapter 3

Ionised absorber outflows in AGN

The first warm absorber identification was reported by Halpern (1984) from observations of the RQQ MR 2251-178 with the Einstein Observatory. Halpern gave a possible explanation for the cause of the observed variable X-ray absorption in this object by invoking absorption by warm photoionised gas rather than cold clouds. The term “warm absorber” was introduced by him as a shorthand to denote the fact that the temperature of the photoionised plasma (∼ 10^5 K) is lower than in the case of a collisionally-ionised thermal plasma of similar ionisation level.

In the days of ROSAT and ASCA, warm absorbers were found through the putative detection of K-shell absorption edges of O vii and O viii ions at 0.74 keV and 0.87 keV, respectively. These edges were first found in the ROSAT Position Sensitive Proportional Counter (PSPC) spectrum of MCG –6-30-15 by Nandra and Pounds (1992). For examples of other early studies of AGN warm absorbers using ROSAT see Nandra et al. (1993) and Turner et al. (1993). The spectral capabilities of ASCA allowed more detailed studies of these edges, such as those by Reynolds (1997a) and George et al. (1998). However, the instruments used at that time had insufficient spectral resolution to measure any details, such as the presence and parameters of narrow absorption lines. With the advent of high-resolution soft X-ray spectroscopy, enabled by the grating instrumentation onboard XMM-Newton and Chandra, a major leap forward in the study of AGN outflows has taken place. It all started with the Chandra Low Energy Transmission Grating Spectrometer (LETGS) discovery of numerous blue-shifted narrow absorption lines generated in a photoionised, outflowing gas, identified in the spectrum of NGC 5548 by Kaastra et al. (2000); this was followed by the identification of similar features in a number of AGN and the
Photoionisation dominates the physics of the warm absorbing material because of its observed high ionisation state and its proximity to the intense high-energy emission of the AGN, which has a significant effect on the ionisation and thermal structure of the warm absorber gas. The physics of the warm absorber plasma in X-ray photoionisation equilibrium is discussed in the following section.

3.1 X-ray photoionised plasmas

If an electron in an atom receives sufficient energy from outside, it will escape from the atom. This process, a bound-free transition, is called ionisation. The incoming energy may be in the form of a photon of sufficient energy (e.g. X-ray) to free an electron and this process is referred to as photoionisation. Thus the photon is absorbed by the atom and an electron is ejected. In photoionisation, the energy of the photon needs to be at least equal to or greater than the ionisation potential. This photoionisation threshold energy is denoted by $\chi$. Let the photon energy be $h \nu$ and the photoionisation cross-section $\sigma_{\text{ph}}$. For $h \nu < \chi$, photoionisation is not possible and the cross-section $\sigma_{\text{ph}}$ is zero. At $h \nu = \chi$, photoionisation is allowed and the cross-section $\sigma_{\text{ph}}$ jumps to a finite value $\sigma_{\text{th}}$, which is the photoelectric absorption cross-section at threshold. This jump is known as the photoelectric absorption edge, so $\chi$ is the energy of the edge. For $h \nu > \chi$, the cross-section $\sigma_{\text{ph}}$ declines from the $\sigma_{\text{th}}$ value; note that contrary to ionisation by an electron, in photoionisation the inner-shell (i.e. K-shell) has the largest cross-section. As shown by Daltabuit and Cox (1972), the K-shell photoionisation cross-sections for H-like and He-like ions (such as O viii and O vii) at $h \nu > \chi$ is approximately

$$\sigma_{\text{ph}} \approx \sigma_{\text{th}} \left( \frac{\chi}{h \nu} \right)^{3.0}$$

The photoionisation cross-sections, widely used in various codes, are provided by the calculations of Verner and Yakovlev (1995). They present a uniform and complete set of analytic fits to the Hartree-Dirac-Slater theoretical calculations of the photoionisation cross-sections at $h \nu > \chi$; their fits demonstrate high level of agreement between theory and experimental calculations of the cross-sections up to energies of 100 keV. Verner and Yakovlev have obtained fit parameters for the photoionisation cross-sections of all shells and subshells of atoms/ions of elements.
3.1. X-ray photoionised plasmas

from H to Zn. Using their results, I have produced a plot of the K-shell photoionisation cross-sections for H-like and He-like ions of C, N and O, shown in Fig. 3.1 displaying the cross-sections at the K-edges of these ions (which are located in the soft X-ray energy band) and their decline towards higher energies.

In photoionisation equilibrium (PIE), the ionisation structure is determined by the balance between photoionisation and recombination. The ionisation balance equation can be written as

\[ n_i \beta_i = n_{i+1} n_e \alpha_{i+1}(T) \] (3.2)

where \( n_i \) is the density of the atoms in the \( i \)-th state of ionisation (i.e. with \( i \) electrons removed), \( n_{i+1} \) is the density of the ionised atoms after one additional ionisation from state \( i \) to \( i + 1 \), \( n_e \) is the electron density, \( \beta_i \) is the photoionisation rate from state \( i \) to state \( i + 1 \), \( \alpha_{i+1} \) is the recombination rate coefficient from state \( i + 1 \) to \( i \). The recombination term \( \alpha_{i+1} \), which is a function of the plasma temperature \( T \), includes both the radiative and dielectric recombinations. The photoionisation rate \( \beta_i \) is related to the photoionisation cross-section \( \sigma_{ph} \) as

\[ \beta_i = \int_{\nu_{th}}^{\infty} F_\nu \frac{\sigma_{ph}}{h\nu} \, d\nu \] (3.3)

where \( \nu_{th} \) is the photoelectric threshold frequency, and \( F_\nu \) is the flux density of the ionising continuum emission as a function of \( \nu \), in units of erg cm\(^{-2}\) s\(^{-1}\) Hz\(^{-1}\). The flux density \( F_\nu \) is given by

\[ F_\nu = \frac{L_\nu}{4\pi r^2} = \frac{L}{4\pi r^2} f_\nu \] (3.4)

where \( L_\nu \) is the luminosity of the ionising source as a function of \( \nu \) (in erg s\(^{-1}\) Hz\(^{-1}\)), \( L \) is the luminosity of the ionising source over the 1–1000 Ryd band (in erg s\(^{-1}\)), \( r \) the distance between the ionised gas and the ionising source (in cm) and \( f_\nu \) is a normalised spectral function, \( \int f_\nu \, d\nu = 1 \), containing the details of the spectral shape of the irradiating continuum. Substituting Eq. (3.4) into Eq. (3.3) gives

\[ \beta_i = \frac{L}{r^2} \int_{\nu_{th}}^{\infty} f_\nu \frac{\sigma_{ph}}{4\pi h\nu} \, d\nu \] (3.5)

which can be abbreviated as

\[ \beta_i = \frac{L}{r^2} \Phi_i \] (3.6)
Substituting Eq. (3.6) back into the ionisation balance equation, Eq. (3.2), gives

\[
\left( \frac{n_{i+1}}{n_i} \right) = \left( \frac{L}{n_e r^2} \right) \frac{\phi_i}{\alpha_{i+1}(T)}
\]  

(3.7)

At this point the ionisation parameter \( \xi \) (Tarter et al. 1969) is introduced which is defined as

\[
\xi \equiv \frac{L}{n_e r^2}
\]  

(3.8)

where \( n_e \) is in units of cm\(^{-3}\) and so \( \xi \) is in units of erg cm s\(^{-1}\). This formulation allows us to conveniently embody the three unknown environmental parameters \( L \), \( n_e \) and \( r \), into a single parameter \( \xi \). For a plasma in photoionisation equilibrium, the ionisation parameter \( \xi \) is commonly used to quantify its ionisation state. So Eq. (3.7) can be re-written as

\[
\left( \frac{n_{i+1}}{n_i} \right)_{\text{PIE}} = \left( \frac{\phi_i}{\alpha_{i+1}(T)} \right) \xi
\]  

(3.9)
In addition, the ionic density can be expressed as \( n_i = A_{\text{elem}} f_i n_H \), where \( A_{\text{elem}} \) is the abundance of the element relative to hydrogen, \( f_i \) is the ion fraction and \( n_H \) is the hydrogen density.

After photoionisation by a photon of energy \( h\nu \), the freed electron possesses a kinetic energy \( h\nu - h\nu_{\text{th}} \). Successive electron-electron collisions distribute this energy throughout the electron population according to a thermal distribution; in other words, the kinetic energy is thermalised into the photoionised plasma. For ions seen in the X-ray, photoionisation is the primary heating contribution and radiative recombination is the primary cooling contribution. The equilibrium temperature \( T \) of the photoionised plasma is determined by the solution of the energy balance equation, where the rate of the energy injection into the plasma due to photoionisation is set equal to the rate of the energy loss from the plasma due to radiative recombination (i.e. radiation). So the energy balance equation is given by

\[
\sum_{\text{elem},i} n_i \beta_i (h\nu - h\nu_{\text{th}}) = \sum_{\text{elem},i} n_{i+1} n_e \alpha_{i+1}(T) k_B T
\]  

(3.10)

where the summations are over all elements and ion states.

Given the specification of the ionisation parameter \( \xi \), the self-consistent solution of the ionisation balance equation (Eq. 3.9) and energy balance equation (Eq. 3.10) yield the \( f_i(\xi) \) values for all the elements, and \( T(\xi) \). Photoionisation codes, such as cloudy\(^\dagger\) (Perland et al. 1998) and xstar\(^\ddagger\) (Bautista and Kallman 2001), are used to calculate these quantities using realistic elemental abundances. The photoionisation codes compute \( \phi_i \) by using the extensive database of photoionisation cross-sections \( \sigma_{\text{ph}} \) and the spectral shape function \( f_\nu \) (i.e. the shape of the SED of the ionising source), which is input into the code by the user. So the physical state of the photoionised gas under the assumption of photoionisation and thermal equilibrium is computed. The photoionisation codes take into account many different elements and a vast body of atomic physics processes, so other heating/cooling mechanisms (albeit less dominant than photoionisation/recombination) are also included, such as Auger ionisation, collisional ionisation, bremsstrahlung and Compton scattering.

\(^\dagger\) http://www.nublado.org  
\(^\ddagger\) http://heasarc.gsfc.nasa.gov/xstar/xstar.html
3.2 Diagnostics of X-ray photoionised plasmas

In most astrophysical systems, some form of equilibrium most likely applies, in which there is a balance between competing processes, e.g., heating and cooling, ionisation and recombination, excitation and de-excitation, etc. The nature of the equilibrium has important effects on the emergent spectrum. For example, there are spectroscopic diagnostics for distinguishing photoionisation equilibrium from collisional ionisation equilibrium (sometimes called coronal equilibrium). Collisional ionisation refers to ionisation of an atom induced by the collision with an energetic electron.

The gas in a photoionised plasma is “over-ionised” at a given electron temperature than it would be in a collisionally ionised plasma. Thus one important difference between a coronal plasma and a photoionised plasma is that $k_B T \sim \chi \sim \Delta E$ for a coronal plasma, whereas $k_B T \ll \chi$ and $\ll \Delta E$ for a photoionised plasma, where $\chi$ is the ionisation potential and $\Delta E$ the threshold energy for excitation. So in photoionised plasmas, electrons have insufficient energy to collisionally excite X-ray lines. In a photoionised plasma, the excitation of lines is dominated by radiative recombination and photoexcitation as opposed to collisional excitation from the ground state in a coronal plasma. As a consequence, high-resolution X-ray spectra of X-ray photoionised plasma present different features from those of collisionally ionised plasma with similar ion concentrations.

3.2.1 Notation for atomic electron configurations and energy levels

The energy state of an atom or ion is specified by a set of quantum numbers, commonly described as

$$n (l\text{-symbol})^q \ldots ^{2S+1}(L\text{-symbol})^P_j$$

(3.11)

where $n (l\text{-symbol})^q \ldots$ denotes the electron configuration and the corresponding energy level is described by the $^{2S+1}(L\text{-symbol})^P_j$ term. $n$ is the principal quantum number which specifies the main energy level (shell) of an atom. For $n = 1, 2, 3, \ldots$, the shells are referred to as K-shell, L-shell, M-shell, etc. $l$ is the orbital quantum number which describes the subshell and gives the magnitude of the electron orbital angular momentum $\vec{l}$ ($0 \leq l \leq n - 1$). For $l = 0, 1, 2, \ldots$, the subshells are denoted by the symbols $s$, $p$, $d$, etc. $q$ represents the number of electrons in the subshell $l$; the maximum number of electrons which can be placed in a subshell is given by
2(2l + 1); this gives maximum of 2 electrons in s, 6 electrons in p, 10 electrons in d, etc. The parity \( P = (-1)^{\sum p_{li}} \), is denoted by an \( o \) for odd, and omitted if even.

The angular momentum of an electron can be written as \( \vec{j} = \vec{l} + \vec{s} \), where \( \vec{l} \) is the orbital angular momentum and \( \vec{s} \) the intrinsic angular momentum (spin). In an atom with more than one electron, the energy level structure is characterised by the combination of the angular momenta (LS coupling), given by the total angular momentum \( \vec{J} = \vec{L} + \vec{S} \), where \( \vec{L} = \sum \vec{l}_i \) and \( \vec{S} = \sum \vec{s}_i \). The associated quantum numbers, \( L, S \) and \( J \) are used in the energy level term of expression (3.11). The total angular momentum quantum number \( J \) takes a range \(|L - S| \leq J \leq |L + S|\).

For \( L = 0, 1, 2 \ldots \), the levels are denoted by the symbols S, P, D, etc. The \( 2S + 1 \) is the multiplicity of the spin, which gives the number of fine-structure levels for a given \( L \).

### 3.2.2 Warm absorber/emitter diagnostics with He-like ions

Figure 3.2 (from Porquet and Dubau 2000) shows a Grotrian diagram (which is used to show the transitions between energy levels in an atom, taking into account the specific selection rules related to changes in angular momentum of the electron) for a He-like ion. The transitions forming the He-like triplet are the resonance line \( \nu (1s^2 1S_0 - 1s 2p 1P_1) \), the intercombination lines \( x \) and \( y \) \((1s^2 1S_0 - 1s 2p 3P_{2,1}, \) respectively) and the forbidden line \( z \) \((1s^2 1S_0 - 1s 2s 3S_1) \). For the analysis of solar coronae, Gabriel and Jordan (1969) first proposed that the relative intensities of the He-like resonance, intercombination and forbidden lines can be used for temperature and density diagnostics. They introduced the ratios, dependent on electron density \( n_e \) and electron temperature \( T_e \),

\[
\mathcal{R}(n_e) = \frac{z}{x + y} \quad (3.12)
\]

\[
\mathcal{G}(T_e) = \frac{z + (x + y)}{w} \quad (3.13)
\]

where \( w, x + y \) and \( z \) stand for the intensities of the resonance, intercombination and forbidden lines, respectively. These line ratios are widely used for density and temperature diagnostics of coronal (collisional) plasmas. These diagnostics have also been extended to study photoionised plasmas, to determine the ionisation processes involved in the plasma (total photoionisation or partial photoionisation with additional collisional ionisation), as well as the density and the electronic temperature. For example, Porquet and Dubau (2000) have computed and compared \( \mathcal{R}(n_e) \)
3.2. Diagnostics of X-ray photoionised plasmas

3.2.1. Line Ratios of He-like Ions

Fig. 3.2: A Grotrian diagram showing He-like transitions between the energy levels. The resonance (w), intercombination (x, y) and forbidden (z) transitions of the He-like triplet are indicated. The upward solid arrows correspond to collisional excitation transition; the upward dashed arrows correspond to photoexcitation transitions; the downward dashed arrows correspond to radiative transitions, including the 2-photon continuum emission (broken arrow) from \( ^1S_0 \) of \( n = 2 \) shell to the ground level. The thick dot-dashed downward arrows correspond to recombination (radiative and dielectric) plus cascade processes. Figure taken from Perquet and Dubau (2000).

and \( \mathcal{G}(T_e) \) for six He-like ions (Cv, N\textsc{vi}, O\textsc{vii}, Ne\textsc{ix}, Mg\textsc{xii} and Si\textsc{xiii}) under collisional, photoionisation and hybrid conditions. The O\textsc{vii} triplet is particularly useful as the lines occur in a convenient part of the X-ray band, at 21.6 Å (w), 21.8 Å (x + y) and 22.1 Å (z), in the high-sensitivity detection range of current spectrometers such as RGS; also it is usually less affected by blending with the warm absorber lines compared to other He-like triplets in the X-ray band, such as Ne\textsc{ix} and Mg\textsc{xii} at higher energies. Figure 3.3 shows an example of an O\textsc{vii} triplet theoretical spectrum (left) and the line ratio \( \mathcal{R} \) as a function of \( n_e \) (right) at different \( T_e \) in a purely photoionised plasma. Although the radiative transition probability for the forbidden line is very small, in a low density plasma (e.g. \( n_e \lesssim 10^{10} \) cm\(^{-3} \) for O\textsc{vii}), collisional excitation transitions from \( ^3S_1 \) to the \( ^3P \) levels are so rare that the \( ^3S_1 \) state can radiatively decay to the \( ^1S_0 \) ground state. In a high density plasma (e.g. \( n_e \gtrsim 10^{12} \) cm\(^{-3} \) for O\textsc{vii}), collisional excitation dominates and the forbidden line disappears and thus \( \mathcal{R} \) gets close to zero.
3.2. Diagnostics of X-ray photoionised plasmas

Fig. 3.3: Left: theoretical spectrum of O\textsc{vii} triplet lines in a purely photoionised plasma with electron density $n_e = 10^{10}$ cm$^{-3}$ and electron temperature $T_e = 10^5$ K, shown at the spectral resolution of RGS. $z$, $x+y$ and $w$ mark the forbidden, intercombination and resonance lines, respectively. Right: the line ratio $R$ as a function of $n_e$ for O\textsc{vii} at different $T_e$ in a purely photoionised plasma. The figures are taken from Porquet and Dubau (2000).

The He-like triplet diagnostic is often applied to the warm absorber/emitter in AGN to obtain information about its density. For example, Collinge et al. (2001) have identified the forbidden and intercombination emission lines of both O\textsc{vii} and Ne\textsc{iix} in NGC 4051. The ratio $R$ is found to be about 5. Since the resonance emission lines are not detected, and their flux is lower than the intercombination line flux, they report the forbidden-to-resonance line ratio $z/w$ has to be $\gtrsim 4$. Such a high $z/w$ ratio implies that the warm emitter is a photoionisation-dominated plasma and the upper limit on its temperature is $10^6$ K. Using this observed ratio and the theoretical calculations of Porquet and Dubau (2000), they obtain an upper-limit of $4 \times 10^{10}$ cm$^{-3}$ for the electron density $n_e$. In NGC 4593, McKernan et al. (2003) have detected only weak forbidden emission lines of O\textsc{vii} and Ne\textsc{iix}, which indicate an origin in a photoionised plasma. They estimate an upper limit of $R < 3$ for Ne\textsc{iix} and $R < 10$ for O\textsc{vii}; these constraints imply $n_e < 2 \times 10^{12}$ cm$^{-3}$ and $n_e < 8 \times 10^{10}$ cm$^{-3}$, respectively, using Porquet and Dubau (2000) calculations. Schurch et al. (2004) have detected triplet emission lines of N\textsc{vi}, O\textsc{vii} and Ne\textsc{iix} in the RGS spectrum of NGC 4151. The $G$ ratios imply an electron temperature of $\lesssim 10^5$ K, consistent with the electron temperatures derived from the properties of the observed radiative recombination continua (see Sect. 3.2.3). The $R$-ratio of N\textsc{vi} and O\textsc{vii} imply
3.3. Thermal stability in photoionised plasma

\( n_e \sim 10^8 - 10^9 \text{ cm}^{-3} \) and the \( R \)-ratio of Ne IX implies \( n_e \sim 10^{10} - 10^{11} \text{ cm}^{-3} \). The line ratios (in particular for O VII, which is both the strongest and the least confused of the He-like triplets) strongly suggest a photoionised plasma. In Sect. 5.5.3, the detection of an O VII forbidden line in the RGS spectrum of NGC 3516 is reported.

3.2.3 Radiative Recombination Continua

Radiative recombination is the process by which an ion in ionisation state \( i + 1 \) captures a free electron and changes to state \( i \), which is accompanied by emission of a photon. Since the free electrons in the plasma will have a thermal (Maxwellian) energy distribution, recombination of free electrons onto the ground state of ions leads to the generation of photons with a range of energies: the product of this is the so-called radiative recombination continua (RRC). The energy of a RRC photon is \( \epsilon = k_B T + \chi \), where \( k_B T \) is the initial energy of the electron and \( \chi \) is the ionisation potential of the level into which the free electron is captured. The width of the RRC is approximately \( \Delta \epsilon \approx k_B T \), thus, in photoionised plasmas \( \Delta \epsilon / \epsilon \approx k_B T / \chi \ll 1 \), which means the RRCs are narrow emission features, allowing them to be contrasted against the underlying continuum spectrum produced by the X-ray source. However, for a coronal plasma, the electrons are at a high temperature with a wide range of energies, so the RRCs will be broad and shallow, making them difficult to distinguish from the underlying continuum. Using the high-resolution grating spectrometers onboard XMM-Newton and Chandra, there have been clear detections of the RRC features. For example, the spectrum of the Seyfert-2 galaxy NGC 1068 as observed by the RGS shows clear evidence of narrow RRC features (Kinkhabwala et al. 2002), indicating an electron temperature of a few eV, characteristic of a photoionised plasma. The spectrum of NGC 1068 is rich in emission lines, especially H-like and He-like lines of C, N, O and Ne. This is because, while in the Seyfert-1 view the warm absorber is seen through its absorption of the intrinsic nuclear continuum, in the Seyfert-2 view the intrinsic continuum is highly absorbed by the dusty torus, allowing for the line-rich emission of the warm absorbing medium (located in the ionisation cone) to be observed.

3.3 Thermal stability in photoionised plasma

X-ray photoionised plasma can be thermally unstable in certain regions of the ionisation parameter space. This can be investigated by means of an “S-curve” diagram:
3.3. Thermal stability in photoionised plasma

this is a plot of the temperature of the plasma, derived by solving the energy balance equation (Eq. 3.10), versus the pressure form of the ionisation parameter, \( \Xi \), introduced by Krolik et al. (1981). The parameter \( \Xi \), which describes the ionisation equilibrium, is defined as

\[
\Xi \equiv \frac{F}{n_e k_B T c}
\]  

(3.14)

where \( F \) is the flux of the ionising source between 1–1000 Ryd (in erg cm\(^{-2}\) s\(^{-1}\)), \( k_B \) the Boltzmann constant, \( T \) the plasma temperature and \( n_e \) is the electron density in cm\(^{-3}\) (as in Eq. 3.8). This expression assumes the ionising radiation is confined to a small solid angle and is normally incident upon the gas cloud. \( F/c \) is the pressure of the ionising radiation. Since \( F = L/4\pi r^2 \), Eq. (3.14) can be re-written as

\[
\Xi = \frac{L}{4\pi r^2 n_e k_B T c}
\]  

(3.15)

Substituting Eq. (3.8) into Eq. (3.15) gives

\[
\Xi = \frac{\xi}{4\pi k_B T c} \approx 19222 \frac{\xi}{T}
\]  

(3.16)

An example of an S-curve (computed as part of my work in Chapter 7) is shown in Fig. 3.4. To obtain \( T(\Xi) \), I ran cloudy for a photoionised gas with Lodders et al. (2009) abundances irradiated with the SED of Mrk 509. On the curve itself, the heating rate is equal to the cooling rate, so the gas is in thermal balance. To the left of the curve, cooling dominates over heating, whilst to the right of the curve, heating dominates over cooling. On branches of the S-curve which have positive gradient, the photoionised gas is thermally stable. Small perturbations upward in temperature increase the cooling, whereas small perturbations downward in temperature increase the heating. However, on the branches with negative gradient (as indicated in Fig. 3.4), the photoionised gas is thermally unstable, in this case,

\[
\left( \frac{\partial(C - H)}{\partial T} \right)_\Xi < 0
\]  

(3.17)

where \( C \) represents the complete set of cooling processes and \( H \) represents the complete set of heating processes. A small perturbation upward in temperature increases the heating, causing further temperature rise, whereas a small perturbation downward increases the cooling. The instability arises because of ionisation through various atomic shells, which acts as a type of phase transition. Depending on how the effects of various heating and cooling processes are computed by codes such as
3.4 High-resolution X-ray spectroscopy

Before the advent of high-resolution X-ray spectrometers, X-ray absorption by ionised outflows was detected using low-resolution instruments only through the measurements of broad and blurred flux dips; at the time, these were interpreted...
3.4. High-resolution X-ray spectroscopy

Fig. 3.5: Continuum (K-edge) and line (Ly-α) absorption spectrum of a slab of O\textsc{viii} ions with column densities indicated inset. The spectra illustrate that O\textsc{viii} Ly-α absorption signature is more prominent than the O\textsc{viii} K-edge for lower column densities, and thus a better indicator of absorption. Figure taken from Jelle Kaastra & Frank Verbunt notes.

as being caused by continuum absorption (e.g. O\textsc{vii} and O\textsc{viii} K-shell absorption edges). However, at high spectral resolution, narrow X-ray absorption lines are also detected, which in fact offer a more sensitive tool for the study of ionised outflows, even with weak absorption. For example, as illustrated in Fig. 3.5, for an O\textsc{viii} column density of $10^{17}$ cm$^{-2}$ ($10^{21}$ m$^{-2}$ curves in the figure), the absorption edge has a low optical depth (about 1%) and is a weak feature, whereas for the same column density, the core of the O\textsc{viii} line is already saturated, providing clearer diagnostics of absorption.

The advent of X-ray observatories with high spectral resolution and sensitivity, such as *XMM-Newton*’s RGS and *Chandra*’s Low Energy Transmission Grating Spectrometer (LETGS) and High Energy Transmission Grating Spectrometer (HETGS), strongly demands spectral codes with a high level of accuracy and detail to fit complicated spectra of astrophysical plasmas. Since 1992, one such software package, called SPEx\footnote{http://www.sron.nl/spex}, has been developed by the SRON institute (Kaastra et al. 1996). The code incorporates many models for the computation of emission and absorption spectra, and associated physical parameters, for different types of astrophysical plasmas, such as those relevant to photoionised warm absorbers in AGN.

As described in Sect. 3.1, photoionisation codes such as CLOUDY compute the equilibrium ion column densities and temperature as a function of the ionisation...
3.4. High-resolution X-ray spectroscopy

parameter \( \xi \), based on the SED of the ionising source and the assumed elemental abundances of the photoionised gas. The results yielded by \textsc{cloudy} runs are then used in the \textsc{spex} code for fitting the high-resolution spectra of warm absorbers. In the recent versions of the \textsc{spex} package, the auxiliary program \textsc{xabsinput}, is used to convert the \textsc{cloudy} output into an input file, containing the temperature and ionic column densities as a function of \( \xi \), for the \textsc{xabs} photoionised absorption model of \textsc{spex}. So the \textsc{xabs} model calculates the transmission through a slab of photoionised gas where all ionic column densities are linked in a physically consistent fashion through the \textsc{cloudy} photoionisation model. In the \textsc{xabs} modelling of the high-resolution spectra of warm absorbers, the ionisation parameter (\( \xi \)), the equivalent hydrogen column density (\( N_{\text{H}} \)) of the warm absorber, its flow and RMS velocities are fitted in \textsc{spex}.

Sometimes it is useful to identify and characterise the absorption lines of the warm absorber before modelling with a photoionisation model. For this purpose, the \textsc{slab} model in \textsc{spex} is used, which calculates the transmission through a slab of material with adjustable ionic column densities. The advantage of this model is that a spectrum can be fitted without any knowledge of the ionisation balance of the plasma. So using the \textsc{slab} model one can get a measure of the column density, its flow and RMS velocities of individual ions independently, especially those with the clearest absorption lines in the spectrum. After a spectral fit has been made, the observed column densities are then interpreted in a physically self-consistent way by modelling with the realistic \textsc{xabs} photoionisation model. In the \textsc{xabs} model the column densities of the ions are not independent quantities, but are linked, based on the ionisation balance computations of \textsc{cloudy} or \textsc{xstar}. So in the \textsc{xabs} model, all the relevant ions are taken into account, including those that would be detected only with marginal significance or not detected at all with the \textsc{slab} model; note that the combined effect of many weak absorption features can be spectrally significant. Of course, if the real ionisation balance of the source is different from the computed ionisation balance, then \textsc{xabs} fails to give an acceptable fit to the warm absorber spectrum.

The effects of the Galactic neutral absorption in the interstellar medium (ISM) are included in my modelling by applying the \textsc{hot} model in \textsc{spex}. This model calculates the transmission of a plasma in collisional ionisation equilibrium. For a
3.5 High-resolution X-ray observations of warm absorbers

given temperature and set of abundances, the model calculates the ionisation balance and then determines all the ionic column densities by scaling to the prescribed total hydrogen column density. The transmission includes both continuum and line opacity. To mimic the transmission of a neutral plasma in collisional ionisation equilibrium (such as the ISM of the Galaxy), the temperature of the plasma is set to 0.5 eV. For a specified right ascension and declination, the Galactic hydrogen H\textsc{i} column density in our line of sight towards the AGN is set to the value derived by Galactic H\textsc{i} map surveys, such as that of Dickey and Lockman (1990) or the Leiden/Argentine/Bonn (LAB) Survey of Galactic H\textsc{i} (Kalberla et al. 2005).

The spex atomic data (such as the absorption cross-sections) are mostly taken from Verner and Yakovlev (1995) for continuum opacities and Verner et al. (1996) for line opacities and wavelengths. spex also has its own additional database for K-shell, L-shell and M-shell transitions obtained from various sources; for information about the atomic database used in spex and references therein, see the spex reference manual (Kaastra et al. 2012a).

3.5 High-resolution X-ray observations of warm absorbers

High-resolution X-ray observations of many Seyfert-1 galaxies and some quasars show evidence of absorbing photoionised gas in our line of sight towards the active nucleus. Using the literature available so far, I have compiled a list of all the AGN which are reported to have warm absorbers, detected in high-resolution spectra with their warm absorbers modelled. As shown in Table 3.1 there are 34 such AGN with warm absorbers (observed with XMM-Newton and/or Chandra), consisting of 20 broad-line Seyfert-1 galaxies, 5 narrow-line Seyfert-1 galaxies, 5 radio-quiet quasars, 2 blazars, 1 broad-line radio galaxy and 1 Seyfert-2 galaxy. Results from different works on one object are also presented when different instruments have been used. In cases where there are multiple studies of an object, preference has been given to those works which have used high-resolution spectroscopy and proper photoionisation modelling of the ionised outflows. The compiled results are presented in Table 3.1 in which the ionisation parameter, column density and outflow velocity for each of the warm absorber phases are given. The type of AGN, redshift, the name of the instrument and the reference paper are also given for each AGN.
Table 3.1: Main parameters of the ionised X-ray outflows detected in high-resolution spectra of AGN. Table continued next page.

<table>
<thead>
<tr>
<th>Object</th>
<th>Type</th>
<th>$z$</th>
<th>Ionised outflows parameters</th>
<th>Flow $v$</th>
<th>Instrument</th>
<th>Reference</th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\log \xi$</td>
<td>$N_H$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Phases 1, 2, ...</td>
<td>Phases 1, 2, ...</td>
<td>Phases 1, 2, ...</td>
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</tr>
<tr>
<td>3C 382</td>
<td>BLRG</td>
<td>0.058</td>
<td>2.69</td>
<td>320</td>
<td>−1200</td>
<td>RGS</td>
</tr>
<tr>
<td>”</td>
<td>”</td>
<td>”</td>
<td>2.45</td>
<td>13</td>
<td>−840</td>
<td>HETGS</td>
</tr>
<tr>
<td>Ark 564</td>
<td>NLSy1</td>
<td>0.0247</td>
<td>−0.86, 0.87, 2.56</td>
<td>0.89, 2.41, 6.03</td>
<td>+20, −40, −10</td>
<td>RGS</td>
</tr>
<tr>
<td>ESO 113-G010</td>
<td>Sy1.8</td>
<td>0.026</td>
<td>2.3, 3.2</td>
<td>50, 160</td>
<td>−700, −1100</td>
<td>RGS</td>
</tr>
<tr>
<td>ESO 323-G077</td>
<td>Sy1.2</td>
<td>0.0150</td>
<td>log $U$: 2.14, 3.26</td>
<td>190, 1300</td>
<td>−3200, −1700</td>
<td>EPIC</td>
</tr>
<tr>
<td>GB B1428+4217</td>
<td>Blazar</td>
<td>4.72</td>
<td>2</td>
<td>1000</td>
<td>?</td>
<td>EPIC</td>
</tr>
<tr>
<td>H1419+480</td>
<td>Sy1.5</td>
<td>0.0723</td>
<td>1.15−1.30</td>
<td>50</td>
<td>?</td>
<td>EPIC</td>
</tr>
<tr>
<td>IC 4329A</td>
<td>Sy1.2</td>
<td>0.0161</td>
<td>−1.37, 0.56, 1.92, 2.70</td>
<td>13, 3, 66, 20</td>
<td>0, −200, −100, +20</td>
<td>RGS</td>
</tr>
<tr>
<td>IRAS 05078+1626</td>
<td>Sy1.5</td>
<td>0.0179</td>
<td>2.5</td>
<td>13000</td>
<td>?</td>
<td>EPIC/RGS</td>
</tr>
<tr>
<td>IRAS 18325-5926</td>
<td>Sy2</td>
<td>0.020</td>
<td>1.58, 2.35</td>
<td>61, 38</td>
<td>−400, −400</td>
<td>HETGS</td>
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<tr>
<td>IRAS 13349+2438</td>
<td>RQQ</td>
<td>0.108</td>
<td>0.225</td>
<td>20, 250</td>
<td>−420, +20</td>
<td>RGS</td>
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<tr>
<td>”</td>
<td>”</td>
<td>”</td>
<td>0.75−1.75 (AMD)$^e$</td>
<td>120</td>
<td>−300</td>
<td>HETGS</td>
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</tbody>
</table>

$^a$ The redshift values are all taken from NED and rounded according to the errors given there.

$^b$ Ionisation parameter in units of erg cm s$^{-1}$.

$^c$ Equivalent hydrogen column density of the warm absorber phase in $10^{20}$ cm$^{-2}$.

$^d$ km s$^{-1}$.

$^e$ Absorption measure distribution (see Holczer et al. 2007 for the details of this method).
### Table 3.1: Continued from previous page and continued next page.

<table>
<thead>
<tr>
<th>Object</th>
<th>Type</th>
<th>$z^a$</th>
<th>Ionised outflows parameters</th>
<th>Instrument</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCG −6-30-15</td>
<td>NLSy1</td>
<td>0.0077</td>
<td>log $\xi^b$</td>
<td>$N_H^c$</td>
<td>Flow $v^d$</td>
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<tr>
<td>MR 2251-178</td>
<td>RQQ</td>
<td>0.0640</td>
<td>1.25, 2.5</td>
<td>20, 20</td>
<td>−150, −1900</td>
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<tr>
<td>Mrk 279</td>
<td>Sy1.5</td>
<td>0.0305</td>
<td>0.7, 2.6</td>
<td>0.7, 2.7</td>
<td>−200, −370</td>
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<tr>
<td>Mrk 290</td>
<td>Sy1.5</td>
<td>0.030</td>
<td>1.57, 2.50</td>
<td>11, 32</td>
<td>−1260, −1260</td>
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<tr>
<td>Mrk 304</td>
<td>Sy1</td>
<td>0.0658</td>
<td>0.8, 2.0</td>
<td>200, 900</td>
<td>?</td>
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<tr>
<td>Mrk 509</td>
<td>Sy1.5</td>
<td>0.0344</td>
<td>−0.33, 0.71, 2.01, 0.23, 0.84, 4.8</td>
<td>−13, −13, −319</td>
<td>RGS</td>
</tr>
<tr>
<td>Mrk 704</td>
<td>Sy1.2</td>
<td>0.0290</td>
<td>1.3, 2.7</td>
<td>2.0, 2.7</td>
<td>−1350, −540</td>
</tr>
<tr>
<td>Mrk 766</td>
<td>NLSy1</td>
<td>0.0129</td>
<td>?</td>
<td>?</td>
<td>0</td>
</tr>
</tbody>
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---

*a* The redshift values are all taken from NED and rounded according to the errors given there.

*b* Ionisation parameter in units of erg cm s$^{-1}$.

*c* Equivalent hydrogen column density of the warm absorber phase in $10^{20}$ cm$^{-2}$.

*d* km s$^{-1}$. 

---
### Table 3.1: Continued from previous page and continued next page.

<table>
<thead>
<tr>
<th>Object</th>
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<th>( z^{a} )</th>
<th>Ionised outflows parameters</th>
<th>Flow ( v^{d} )</th>
<th>Instrument</th>
<th>Reference</th>
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<td></td>
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<td>log ( \xi^{b} ) ( \log_{10} N_{H}^{c} ) Phase 1, 2, 3, ...</td>
<td>Phase 1, 2, 3, ...</td>
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<td></td>
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<td>Mrk 841</td>
<td>Sy1.5</td>
<td>0.036</td>
<td>1.5, 3.2</td>
<td>23, 300</td>
<td>0, 0</td>
<td>RGS</td>
</tr>
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<td>NGC 985</td>
<td>Sy1</td>
<td>0.0431</td>
<td>log ( U ): 0.05, 1.31</td>
<td>12, 98</td>
<td>–280, –280</td>
<td>RGS</td>
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<td>&quot;</td>
<td>&quot;</td>
<td>&quot;</td>
<td>log ( U ): –0.12, 1.34</td>
<td>25, 65</td>
<td>–200, –580</td>
<td>HETGS</td>
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<tr>
<td>NGC 3227</td>
<td>Sy1.5</td>
<td>0.0039</td>
<td>1.2, 2.9</td>
<td>11, 24</td>
<td>–420, –2060</td>
<td>RGS</td>
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<td>NGC 3516</td>
<td>Sy1.5</td>
<td>0.0088</td>
<td>0.9, 2.4, 3.0</td>
<td>40, 200, 100</td>
<td>–100, –1500, –900</td>
<td>RGS</td>
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<td>NGC 3783</td>
<td>Sy1.5</td>
<td>0.00973</td>
<td>0.3, 2.4</td>
<td>5.4, 280</td>
<td>–800, –800</td>
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<td>NGC 4051</td>
<td>NLSy1</td>
<td>0.00234</td>
<td>1.0, 3.3, 4.5</td>
<td>2.0, 10.1, 8.1</td>
<td>–400, –630, –680</td>
<td>HETGS</td>
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<td>&quot;</td>
<td>0.23, 2.77, 1.43, 1.0, 29, 11.1</td>
<td>+120, –400, –530,</td>
<td></td>
<td>RGS</td>
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<tr>
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<td>2.52, 2.97</td>
<td>19, 140</td>
<td>–3850, –5880</td>
<td>&quot;</td>
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<td>NGC 4151</td>
<td>Sy1.5</td>
<td>0.0033</td>
<td>log ( U ): –0.27, 1.05</td>
<td>290, 320</td>
<td>–500, –1250</td>
<td>HETGS</td>
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<td>NGC 4395</td>
<td>Sy1.8</td>
<td>0.00106</td>
<td>0.5, 2.6</td>
<td>67, 190</td>
<td>?</td>
<td>EPIC</td>
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</table>

\( ^{a} \) The redshift values are all taken from NED and rounded according to the errors given there.

\( ^{b} \) Ionisation parameter in units of erg cm s\(^{-1}\).

\( ^{c} \) Equivalent hydrogen column density of the warm absorber phase in \(10^{20}\) cm\(^{-2}\).

\( ^{d} \) km s\(^{-1}\).
Table 3.1: Continued from previous page.

<table>
<thead>
<tr>
<th>Object</th>
<th>Type</th>
<th>$z$</th>
<th>Ionised outflows parameters</th>
<th>Instrument</th>
<th>Reference</th>
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<tr>
<td></td>
<td></td>
<td></td>
<td>log $\xi$ $^b$</td>
<td>$N_{H}$$^c$</td>
<td>Flow $v$$^d$</td>
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<td>Phases 1, 2, ...</td>
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<td>NGC 4593</td>
<td>Sy1</td>
<td>0.009</td>
<td>0.5, 2.61</td>
<td>0.6, 16</td>
<td>−380, −400</td>
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<td></td>
<td></td>
<td>2.52</td>
<td>53.7</td>
<td>−140</td>
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<tr>
<td>NGC 5548</td>
<td>Sy1.5</td>
<td>0.0172</td>
<td>0.40, 1.98, 2.69</td>
<td>1.41, 33.1, 47.9</td>
<td>−290, −440, −311</td>
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<td>NGC 7469</td>
<td>Sy1.2</td>
<td>0.01632</td>
<td>0.8, 2.73, 3.56</td>
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<td>PDS 456</td>
<td>RQQ</td>
<td>0.184</td>
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<td>5000</td>
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<tr>
<td>PG 0844+349</td>
<td>RQQ</td>
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<td>3.7</td>
<td>4000</td>
<td>−60000</td>
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<tr>
<td>PG 1211+143</td>
<td>RQQ</td>
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<td>−0.9, 1.7, 3.4</td>
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<td>?, −24000, −24000</td>
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<tr>
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<td></td>
<td>?</td>
<td>10–100</td>
<td>−3000</td>
</tr>
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<td>0.8–1.2</td>
<td>200–316</td>
<td>?</td>
</tr>
<tr>
<td>RE J1034+396</td>
<td>NLSy1</td>
<td>0.042</td>
<td>3.2</td>
<td>40</td>
<td>?</td>
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</table>

$^a$ The redshift values are all taken from NED and rounded according to the errors given there.

$^b$ Ionisation parameter in units of erg cm s$^{-1}$.

$^c$ Equivalent hydrogen column density of the warm absorber phase in 10$^{20}$ cm$^{-2}$.

$^d$ km s$^{-1}$.
3.6 Location of the warm absorbers

From Table 3.1 the warm absorber phases are found to be outflowing with an average flow velocity of $-640 \text{ km s}^{-1}$ for the Seyferts and $-1100 \text{ km s}^{-1}$ for the NLSy1s. However, the median flow velocity is the same for both the Seyferts and NLSy1s: $-400 \text{ km s}^{-1}$. For the RQQs, the average and median flow velocities are $-19100 \text{ km s}^{-1}$ and $-18000 \text{ km s}^{-1}$, respectively. For Seyferts, the average and median $N_H$ values are $3.4 \times 10^{22} \text{ cm}^{-2}$ and $3.4 \times 10^{21} \text{ cm}^{-2}$, respectively. For NLSy1s, the average and median $N_H$ are $2.1 \times 10^{21} \text{ cm}^{-2}$ and $9.1 \times 10^{20} \text{ cm}^{-2}$, respectively. For RQQs, the average and median $N_H$ are $2.0 \times 10^{23} \text{ cm}^{-2}$ and $5.2 \times 10^{22} \text{ cm}^{-2}$, respectively.

A few of the authors quoted in Table 3.1 have used the ionisation parameter $U$ to describe photoionisation equilibrium, which is different from $\xi$ (introduced in Sect 3.1). The ionisation parameter $U$ was first introduced by Davidson (1972) to characterise the ratio of ionising radiation over the electron density, and hence describe the ionisation equilibrium, in a similar fashion to $\xi$ (see Eq. 3.7). The ionisation parameter $U$ was first defined as $U_1 = F_1/h\nu n_e$, where $F_1$ denotes flux density of the ionising source at $h\nu = 1 \text{ Ryd} \approx 13.6 \text{ eV}$, thus $U_1 = F_1/n_e$. However, subsequently the ionisation parameter $U$ has been used in the literature as

$$
U \equiv \int \frac{F_\nu}{h\nu n_e} \, d\nu = \int \frac{L_\nu}{4\pi r^2 h\nu n_e} \, d\nu
$$

(3.18)

where $U$ is integrated over the entire Lyman continuum between 1–1000 Ryd. Sometimes in the literature $U$ is only integrated over the X-ray band (0.1–10 keV) and is then named the X-ray ionisation parameter, $U_X$ (introduced by Netzer 1996). Substituting Eqs. (3.4) and (3.8) into Eq. (3.18), the relationship between $U$ (integrated between 1–1000 Ryd) and $\xi$ is given by

$$
U = \xi \int \frac{f_\nu}{4\pi h\nu} \, d\nu
$$

(3.19)

thus, the spectral function of the ionising source is required in order to convert between $U$ and $\xi$.

3.6 Location of the warm absorbers

From Eq. (3.8), the distance between the warm absorber and the ionising source can be expressed as

$$
r = \sqrt{L/\xi n_e}
$$

(3.20)
Since $L$ can be measured from observations and $\xi$ can be deduced from photoionisation modelling and spectroscopy of the warm absorber, by measuring the density $n_e$, the distance $r$, which is unknown, can be obtained.

There have been a few attempts to directly measure the density $n_e$ using density-sensitive meta-stable lines in some AGN. Using this method in the UV band, the published results display a wide range of distances for different sources: < 0.1 pc in NGC 4151 [Kraemer et al. 2006], ~ 25 pc in NGC 3783 [Gabel et al. 2005], ~ 3.3 kpc in SDSS J0838+2955 [Moe et al. 2009]. However, observations of the lines are difficult as they are often weak and contaminated by other lines, and also it is uncertain whether the derived distances are also applicable to the higher ionised X-ray outflows. In the X-ray band, Kaastra et al. (2004) pioneered this method theoretically and observationally using K-shell absorption of O\textsc{v} under photoionised conditions. However, due to the weak signal detected by Chandra/LETGS from the AGN (Mrk 279), they could not obtain firm measurements of the line and thus the density. To this date, meta-stable lines in the X-ray band have not given a robust measurement of the density yet.

However, there is another good alternative for measuring the density $n_e$. This is through reverberation mapping of the warm absorber. The idea behind this is that as the ionising luminosity of the AGN rises or falls over time, the warm absorber receives larger or smaller amounts of ionising radiation, which results in further ionisation or recombination of the warm absorber gas. Variability of the intrinsic emission thus induces changes in the ionic composition of the nearby warm absorber and hence the transmitted spectrum changes. However, the warm absorber medium does not respond instantaneously to continuum changes as the recombination rate depends on the gas density. How fast the gas responds depends on the recombination timescale $t_{\text{rec}}$, which is a function of density $n_e$. If for instance, a sudden fall in continuum flux is followed by delayed recombination, the measured delay time can be used to calculate the density $n_e$. The recombination timescale $t_{\text{rec}}$ is defined as

$$t_{\text{rec}} = \frac{n_i}{n_{i+1} n_e \alpha_{i+1}(T)}$$

(3.21)

where, similar to Eq. 3.2, $n_i$ and $n_{i+1}$ are the densities of the ions in state $i$ and $i+1$, $n_e$ is the electron density, $\alpha_{i+1}$ is the recombination rate coefficient from state $i+1$ to $i$ and is a function of the temperature $T$. Thus, since $t_{\text{rec}} \propto n_e^{-1}$, by
3.6. Location of the warm absorbers

measuring the recombination timescale one can measure the electron density, and hence the distance $r$ using Eq. (3.20).

Using the ionisation balance equation (Eq. 3.2), since the photoionisation rate per particle $\beta$ (Eq. 3.3) leads to increase the ionisation stage from $i$ to $i+1$ and the recombination rate per particle $n_e \alpha$ to decrease the ionisation stage from $i$ to $i-1$, the time dependence of the relative density $n_i$ of an ion of a given species in ionisation state $i$ is

$$\frac{dn_i}{dt} = (n_{i+1} n_e \alpha_{i+1\rightarrow i}) - (n_i n_e \alpha_{i\rightarrow i-1}) + (n_{i-1} \beta_{i-1\rightarrow i}) - (n_i \beta_{i\rightarrow i+1}) \quad (3.22)$$

The recombination rate coefficient $\alpha$ is a function of the electron temperature $T$ and scales roughly as $T^{-1/2}$ (Osterbrock and Ferland 2006). For each epoch, the equilibrium ion concentrations are calculated using CLOUDY, for the corresponding SED of the ionising source. The photoionisation and recombination rates are also calculated by CLOUDY. Equation (3.22) forms a set of differential equations, which can be solved numerically, to calculate $t_{\text{rec}}$. Figure 3.6 shows an example of recombination timescales for O and Fe ions in a warm absorber as expected in response to the continuum variability of Mrk 509.

An important requirement using the reverberation mapping technique is that the AGN intrinsic emission varies (1) on a suitable timescale and (2) with a sufficient amplitude. For X-ray rapidly variable Seyferts (e.g. MCG –6-30-15 or NGC 4051) the variability timescales of minutes to hours make it impossible to obtain high-resolution spectra of sufficient quality with the current instruments. For example, for a bright Seyfert AGN, the RGS needs an integration time of at least $\sim 50$ ks to obtain a high quality spectrum, so the best candidates are bright Seyferts with variability timescales of a few days. The continuum variability also needs to have sufficient amplitude, otherwise the expected change in the ionic column densities would be too small to be detected significantly.

Such a reverberation measurement was performed as part of a multi-wavelength campaign on the Seyfert-1/QSO Mrk 509 (see Chapter 6). The key for this study was a deep 600 ks time-averaged RGS spectrum ($10 \times 60$ ks XMM-Newton observations), which made it possible to derive accurately the ionisation structure of the outflow. The discrete warm absorber components found by Detmers et al. (2014) were used to calculate the absorber’s time-dependent transmission for dif-
3.6. Location of the warm absorbers

Fig. 3.6: Recombination response times to continuum variations of a typical bright AGN (Mrk 509) for O and Fe in different ionisation stages in a warm absorber at indicated distances from the ionising source. Figure is taken from Kaastra (2008).

Different distances to the central source. From broad-band spectral modelling using OM and EPIC-pn data, the shape of the ionising continuum and its variability during the XMM-Newton campaign were established by Mehdipour et al. (2011) (see Chapter 6); these are important ingredients for the study of the response of the warm absorber to continuum changes. Whilst RGS accurately measures the average ionisation distribution \( N_H(\xi) \) through the measurement of individual ionic column densities, the high throughput of EPIC-pn allows determining the time variations of these column densities by comparing the spectra over the diagnostic region at around 1 keV, where most of the changes in transmission from the warm absorber are expected. The results of this warm absorber reverberation mapping have been published in Kaastra, Detmers, Mehdipour et al. (2012). The distance limits derived for the three main warm absorber components of Mrk 509 are:

- \( r > 70 \) pc \quad (\log \xi \approx 2.0, N_H \approx 4.8 \times 10^{20} \) cm\(^{-2}\)
- \( 5 < r < 33 \) pc \quad (\log \xi \approx 2.8, N_H \approx 5.7 \times 10^{20} \) cm\(^{-2}\)
- \( 5 < r < 21-400 \) pc \quad (\log \xi \approx 3.6, N_H \approx 5.4 \times 10^{21} \) cm\(^{-2}\)

These imply a warm absorber origin in the NLR or the torus region, rather than
3.7 Energetics of the ionised outflows and their contribution to feedback

The mass of a warm absorber phase, assuming spherical outflow is given by

$$M_{WA} = 4\pi r^2 \mu m_p N_H C_g$$  \hfill (3.23)

where \( r \) is the radius of the absorber (i.e. its distance from the SMBH), \( \mu \) is the mean atomic mass per proton (\( \sim 1.4 \) for solar abundances), \( m_p \) is the proton mass, \( N_H \) is the hydrogen column density and \( C_g \) is the global covering fraction and is equal to \( \Omega/4\pi \), where \( \Omega \) is the solid angle subtended by the absorber (see e.g. Krolik and Kriss 2001; Crenshaw et al. 2003). Note here it is assumed that the absorber is uniformly filling the volume within the solid angle covered. Thus, using Eq. (3.23), for a non-accelerating absorber outflowing with velocity \( v \), the mass outflow rate is

$$\dot{M}_{\text{out}} = 4\pi r \mu m_p N_H C_g v$$  \hfill (3.24)

The kinetic energy carried out by the absorber per unit time (i.e. the kinetic luminosity of the absorber) is given by

$$L_{\text{kin}} = \frac{1}{2} \dot{M}_{\text{out}} v^2$$

$$L_{\text{kin}} = 2\pi r \mu m_p N_H C_g v^3$$  \hfill (3.25)

So the energetics of an absorber are dependent on the observables \( N_H \) and \( v \), which can be directly determined from high-resolution spectroscopy, and the less certain quantities \( r \) and \( C_g \). In Sect. 3.6 techniques such as reverberation mapping of the absorber were described for obtaining the distance \( r \). As given in Crenshaw and Kraemer (2012), a number of studies have shown the global covering factor \( C_g \sim 0.5 \), for both UV absorbers (e.g. Dunn et al. 2007) and X-ray absorbers (e.g. Reynolds 1997a). Note that the global covering fraction \( C_g \) is the fraction of intrinsic emission intercepted by the warm absorber, averaged over all
lines of sight, which is different from the covering fraction of an absorber in the line of sight, $C_f$, which in principle can be obtained from spectral fitting (see e.g. Chapter 5 for a partially covering absorber in NGC 3516). The parameter $C_g$ can be determined statistically from a sample of AGN of the same type (e.g. Seyfert-1s), using $C_g = f \langle C_f \rangle$, where $f$ is the fraction of AGN that show intrinsic warm absorption and $\langle C_f \rangle$ the average over all objects of the $C_f$ values for the warm absorber in each object. For example, Crenshaw et al. (1999) find for a sample of 17 Seyfert-1 galaxies, $f = 0.59$ and $\langle C_f \rangle \geq 0.86$, which leads to $C_g \geq 0.51$ for UV absorbers. Another method to determine $C_g$ directly for a given AGN is to compare the strength of emission lines associated with the absorption regions to those predicted from photoionisation modelling assuming full coverage of the continuum source. The ratio of the observed to predicted emission line strengths then gives the $C_g$ for a given source; studies using this method show $C_g = 0.5−1.0$ for X-ray absorbers (Crenshaw et al. 2003).

Crenshaw and Kraemer (2012) have calculated the mass outflow rate and kinetic luminosity for a sample of 6 nearby AGN, which have some of the best studied UV and X-ray absorbers found in the literature, with sufficient constraints on the absorber locations. The studied AGN have moderate bolometric luminosities ($L_{\text{bol}} = 10^{43}−10^{45}$ erg s$^{-1}$). They find the kinetic luminosity, summed over all the absorbers, is $L_{\text{kin}} \approx 0.5−5\% L_{\text{bol}}$ for 3 of the AGN (NGC 3516, NGC 3783 and NGC 4051). Two of the AGN (NGC 4151 and NGC 5548) have $L_{\text{kin}} \gtrsim 0.1\% L_{\text{bol}}$ and one (NGC 7469) has $L_{\text{kin}} \lesssim 0.1\% L_{\text{bol}}$.

Interestingly, feedback models require between $\sim 0.5\%$ (Hopkins and Elvis 2010) and $\sim 5\%$ (Di Matteo et al. 2005) of the bolometric luminosity of an AGN to be converted to kinetic luminosity in order to regulate the growth of a SMBH and its galactic bulge. Thus the UV and X-ray absorber outflows in moderate luminosity AGN (i.e. the Seyferts) have the potential to make significant contribution to the feedback to their environments.
Chapter 4

XMM-Newton and data reduction

4.1 The XMM-Newton observatory

The X-ray Multi-Mirror Mission (XMM-Newton), named in honour of Sir Isaac Newton, was launched on board an Ariane 5 rocket (504) on 10 December 1999 from the European Space Agency (ESA) French Guiana Spaceport. XMM-Newton is a cornerstone mission in ESA’s Horizon 2000 programme. The initial proposal was made to the agency in 1982 and the primary objectives of the mission were first discussed in an ESA workshop in Denmark in 1985. The spacecraft [Jansen et al. 2001], which had a launch mass of 3.8 tonnes, is 10 meters long and with its solar arrays deployed has a span of 16 meters. It carries three X-ray telescopes with CCD X-ray detectors at their foci, and an optical/UV telescope, thus offering simultaneous access to the X-ray and optical/UV bands of the electromagnetic spectrum. XMM-Newton is made up of two large payload modules: the Service Module (SVM) and the Mirror Support Platform (MSP) at one end of the spacecraft, and the Focal Plane Assembly (FPA) at the other end. They are connected by a 6.8 m carbon fibre tube which forms the telescope optical bench.

As shown in Fig. 4.1, the MSP includes three Mirror Modules, two of which are equipped with Reflection Grating Arrays (RGAs) at the back. The Optical Monitor (OM) optical/UV telescope [Mason et al. 2001] and two star-trackers are also located at the same end of the spacecraft. On the FPA reside the two Reflection Grating Spectrometer (RGS) readout cameras [den Herder et al. 2001], the European Photon Imaging Camera (EPIC) pn [Strüder et al. 2001] and MOS [Turner et al. 2001] CCD cameras. The EPIC and RGS instruments are fitted with radiators,
4.1. The XMM-Newton observatory

Fig. 4.1: An open view sketch of the XMM-Newton observatory payload. The three X-ray Mirror Modules, two of which are equipped with the Reflection Grating Arrays, are visible at the lower left on the Mirror Support Platform. The OM telescope is also mounted on the Mirror Support Platform, and is shown behind the lower mirror module. On the right is the Focal Plane Assembly: the back end of the instrument platform with all the X-ray cameras and radiators is shown. Image courtesy of Dornier Satellite System GmbH and ESA, with the labels added by myself.

which cool the CCD detectors via cold fingers. The SVM carries the spacecraft subsystems and associated units providing the necessary resources to the satellite. The SVM is attached to two solar-array wings, the Telescope Sun Shield (TSS) and two S-band antennas mounted on booms.

Each of the three X-ray telescopes consists of 58 Wolter Type-1 grazing incidence mirrors which are nested in a coaxial and confocal configuration (Aschenbach et al. 1987; Jansen et al. 2001). The focal length of the telescopes is 7.5 m, with an angular resolution of about 6 arcsec Full Width Half Maximum (FWHM) and 15 arcsec Half Energy Width (HEW) of the Point Spread Function (PSF). XMM-Newton has the largest effective area of any X-ray telescope built to this date; the total mirror effective area at 1.5 keV is 1550 cm$^2$ for each telescope, i.e., 4650 cm$^2$ in total (XMM-Newton Users Handbook, 2011). Some of the features of the scientific instruments onboard XMM-Newton, which have provided data for this thesis, are described below.
4.1.1 The Reflection Grating Spectrometer

The RGS instrument allows high-resolution \( (E/\Delta E = 100–500) \) measurements in the soft X-ray energy band (6–38 Å, or 0.3–2.1 keV). Its design is optimised for the detection of the K-shell transitions of C, N, O, Ne, Mg, and Si, as well as the L-shell transitions of Fe. The layout of the RGS instrument and geometry of the reflection grating are shown in Fig. 4.2.

Each RGS instrument chain includes a Reflection Grating Array (RGA), which contains 182 identical diffraction gratings (one of the two RGA contains 181 gratings owing to a problem encountered during installation), each measuring about 10 × 20 cm [den Herder et al. 2001]. Each RGA intercepts about half of the total light focused by the associated mirror module, and reflects it to the CCD detectors at the focal plane. The undeflected light passes through and is collected by the EPIC-MOS cameras which are at the primary focus of the two X-ray telescopes with the RGA. The X-ray beam is incident at an angle \( \alpha \) with respect to the plane of the grating, which has triangular grooves tilted at an angle \( \delta \) with respect to that plane (see Fig. 4.2). The gratings are mounted at grazing incidence to the beam in the classical in-plane configuration, in which the incident and diffracted X-rays lie in a plane that is perpendicular to the grating grooves. The radiation is dispersed into angle \( \beta \), and from the position of the X-ray event on the detector the wavelength \( \lambda \) is obtained using the dispersion relation,

\[
ml = d (\cos \beta - \cos \alpha),
\]

where \( m \) is the spectral order \((-1, -2, \ldots)\) and \( d \) is the groove spacing. The spectral resolution of a reflection grating spectrometer is

\[
\Delta \lambda = \frac{d}{m} \sin \alpha \Delta \alpha,
\]

so a high angular resolution \( \Delta \alpha \) and a small grating period \( d \) contribute to a high spectral resolution. The \( \Delta \lambda \) at 15 Å is about 0.06 Å for the first-order RGS1 spectra; Fig. 4.2 shows the first-order and second-order spectral resolution for the two RGS instrument chains.

The diffracted X-rays are detected in single photon counting mode by the RGS Focal Cameras (RFC) with a strip of 9 back-illuminated CCD detectors (similar to those in the EPIC-MOS cameras; see next section) which lie along the curvature...
4.1. The XMM-Newton observatory

Fig. 4.2: Schematic layout of the XMM-Newton RGS instrument. Figure taken from Brinkman et al. (1998). Note angle $\beta$ in Eq. (4.1) is $\beta = \gamma + \delta$, where angles $\gamma$ and $\delta$ are shown above.

of the Rowland circle. The spectrum of an on-axis point source will appear as a line image along the detector array. The position of an X-ray event along the CCD image of the spectrum provides an accurate measure of the energy of the input photon. The length of the CCD strip (253 mm) covers the first-order 6–38 Å wavelength range. The inter-chip gap between two adjacent CCDs is about 0.5 mm. The first and second order spectra, which are overlapping, are separated using the inherent energy resolution of the CCDs. Two CCDs (CCD 7 of RGS 1 and CCD 2 of RGS 2) had an operational failure in year 2000, therefore the 10.5–14.0 Å range in RGS 1 and 20.1–23.9 Å in RGS 2 are unavailable (den Herder et al. 2001). To reduce the dark current and improve general performance, the CCDs are cooled to $-80$ °C. Cooling is accomplished by a two-stage radiator, facing deep space, and by three nested thermal shells around the CCD bench (den Herder et al. 2001). The first shield also contains four internal calibration sources, which produce
4.1. The XMM-Newton observatory

Fig. 4.3: The first-order and second-order spectral resolution of the XMM-Newton RGS1 and RGS2 instrument chains. The curves show the predicted and the data points show the measured spectral resolution (FWHM). Figure taken from den Herder et al. (2001).

Al Kα (1487 eV) and F Kα (676.8 eV) fluorescent emission and illuminate a small area of two CCDs, which is offset in the cross dispersion direction from the source image (den Herder et al. 2001). The wavelength accuracy of the RGS is 7 mÅ, and the maximum effective area (combining RGS1 and RGS2) is about 125 cm² at 15 Å for the first spectral order and about 57 cm² at 10 Å for the second spectral order (XMM-Newton RGS Calibration Status 2011). Fig. 4.4 shows the effective area curves for the two RGS instrument chains; the two failed CCDs and the CCD boundaries can be easily identified.

The RGS instrument has 3 modes of operation: Spectroscopy, High Time Resolution mode and Diagnostic mode. Spectroscopy is the most commonly used mode, in which the 9 CCDs are read out sequentially with a read-out time per CCD of about 0.6 s. In this mode, the positions of the photons along the dispersion axis and perpendicular to this axis are stored, which allows for optimum separation of source and background, thus providing optimum signal-to-noise ratios. The High Time Resolution mode achieves the shortest accumulation time (about 15 ms) if only one CCD is read out; more than one CCD can be used to collect data in this mode, but this increases the accumulation time accordingly. The disadvantage of this mode is the lack of cross dispersion data that can be used to subtract the background. In the
4.1. The XMM-Newton observatory

Fig. 4.4: The first-order and second-order effective area curves of the RGS1 and RGS2 instrument chains. The effective areas are taken from XMM-Newton RGS Calibration Status (2011).

Diagnostic mode, full CCD images are transferred to the ground at low repetition rates, and are used for detailed studies of the CCD performance.

4.1.2 The EPIC-MOS and EPIC-pn cameras

The EPIC consortium provided a set of three X-ray CCD cameras for the three X-ray telescopes on XMM-Newton. Two of the cameras incorporate MOS type CCDs (referred to as EPIC-MOS cameras, Turner et al. 2001) and are located at the focal plane of the two X-ray telescopes which are equipped with the reflection gratings of the RGS. The gratings divert about half of the telescope incident X-ray flux towards the RGS detectors such that about 44% of the original incoming flux reaches the MOS cameras. The other EPIC camera, containing the novel pn-CCDs (referred to as EPIC-pn camera, Strüder et al. 2001), is at the focus of the third X-ray telescope without RGS gratings and thus receives the full photon flux from the telescope without obscuration. The term MOS refers to Metal Oxide Semiconductor
4.1. The XMM-Newton observatory

Fig. 4.5: Photographs of the EPIC-MOS (left) and EPIC-pn (right) CCD arrays. The central MOS CCD is on-axis, and the surrounding 6 CCDs are set above the central device to better approximate the curved focal plane surface. The non-exposed side of the pn CCD array is shown, where the 12 pn CCDs can be seen in the centre of the wafer. Photos courtesy of XMM-Newton SOC, VILSPA.

technology and pn to implanted p-n junction semiconductor technology, which were used in the production of the detectors. Photos of the EPIC-MOS and EPIC-pn CCD chips are shown in Fig. 4.5.

The EPIC cameras perform extremely sensitive imaging observations over a field of view of 30 arcmin and the energy range 0.15–12 keV, with moderate spectral ($E/\Delta E \sim 20–50$) and angular resolution (FWHM $\sim 6$ arcsec, HEW $\sim 15$ arcsec, determined by the telescope) (XMM-Newton Users Handbook 2011). All EPIC CCDs operate in photon counting mode with a fixed, mode dependent frame read-out frequency, producing event lists. This allows for simultaneous imaging and non-dispersive spectroscopy due to the intrinsic energy resolution of the CCD detectors.

Each of the EPIC-MOS cameras contains 7 CCD chips (Type-22 CCDs manufactured by EEV, re-named E2V). The MOS CCD is a three-phase frame transfer device that uses high resistivity silicon and an open electrode structure to obtain a useful quantum efficiency between 0.2 keV and 10 keV. Each CCD has $600 \times 600$ pixels, each $60 \mu m$ square; one pixel covers $1.1 \times 1.1$ arcsec on the sky. The individual CCDs are offset with respect to each other, following closely the slight curvature of the focal surface of the telescopes. Note CCD6 on MOS1 has been switched off due to a hardware failure most likely caused by a micrometeorite impact in March 2005.
The EPIC-pn camera contains a single silicon wafer, integrated with 12 monolithically implanted CCD chips, developed and manufactured in a dedicated semiconductor laboratory of the Max-Planck-Institut für extraterrestrische Physik (MPE), Garching. The CCDs are arranged in four quadrants of three CCDs each. The single CCD, with a dimension of $3 \times 0.98$ cm, has $200 \times 64$ pixels, each $150 \, \mu \text{m}$ square; one pixel corresponds to $4.1 \times 4.1$ arcsec on the sky. The 64 read-out anodes of each CCD are connected via on chip JFETs (Junction Field Effect Transistors) to a 64 channel charge sensitive amplifier (Strüder et al. 2001). The readout of the pn chips is much faster than that of the MOS cameras, because each pixel column has its own readout node. Another important difference is that the pn chips are back-illuminated, while the MOS CCDs are front-illuminated, which affects the detector quantum efficiencies. Quantum efficiency is one of the factors which needs to be taken into account in determining the effective area of the EPIC cameras. MOS CCDs have a poorer low energy response compared to pn CCDs, but have higher spectral resolution and lower background. The quantum efficiency of the EPIC-MOS chips is lower than that of the EPIC-pn CCDs also at higher energies. Figure 4.6 shows the effective area curves of the EPIC-MOS, EPIC-pn and RGS instruments for comparison.

As an X-ray photon is absorbed in a CCD, it produces a charge cloud which is sometimes shared between several adjacent pixels. Thus this splitting of an X-ray event must be recognised and reconstructed into a single photon. The generated X-ray pattern for EPIC is coded as 0 for single-pixel events (i.e. no splitting) and 1-4 for double-pixel events (i.e. two pixel events) depending on their spatial distribution; see e.g. Turner et al. (2001) for more event patterns and details on this. Recommendations on pattern selection for spatial and spectral analysis of EPIC event lists are given in XMM-Newton EPIC Calibration Status (2012).

The EPIC cameras allow several science modes of data acquisition. The EPIC-pn camera can be operated in common modes in all quadrants. The science modes for EPIC are: Full Frame for pn ($26 \times 27$ arcmin, 73 ms time resolution) and MOS ($11 \times 11$ arcmin, 2.6 s resolution), Large Window for pn ($26 \times 13.6$ arcmin, 48 ms resolution) and MOS ($5.5 \times 5.5$ arcmin, 0.6 s resolution), Small Window for pn ($4.4 \times 4.4$ arcmin, 5.7 ms resolution) and MOS ($1.8 \times 1.8$ arcmin, 0.3 s resolution), Timing for pn (0.03 ms resolution) and MOS (1.75 ms resolution) and Burst mode.
4.1. The XMM-Newton observatory

Fig. 4.6: Effective area curves for the three XMM-Newton X-ray telescopes (EPIC-pn, EPIC-MOS and RGS). The effective areas are taken from XMM-Newton Users Handbook (2011).

for pn only (7µs resolution). The EPIC-pn also has an Extended Full Frame mode which uses a longer frame time (i.e. image collection time) than in the normal Full Frame mode. Note that in the case of EPIC-MOS the outer ring of 6 CCDs remain in standard Full Frame imaging mode while the central MOS CCD can be operated separately. The EPIC-pn camera is operated in the same mode in all quadrants for Full Frame, Extended Full Frame and Large Window mode, or just with one single CCD (CCD 0 in quadrant 1) for Small Window, Timing and Burst mode. The choice of mode is based on the extent of the source and its brightness; for bright point sources like AGN, modes with smaller field of view are preferred to improve the readout time resolution and increase the photon pile-up limit. Pile-up refers to the arrival of more than one photon in one pixel before it is read out; it can affect both the PSF and the spectral response of EPIC and should be avoided. There are four aluminised optical blocking filters on each EPIC camera: Thin, Medium and Thick filters, each of which can be used to reduce the optical contamination of the X-ray signal depending on the observed target, and a closed filter to protect the
CCDs from soft protons in orbit.

4.1.3 The Optical Monitor

The OM is a standalone optical/UV telescope, co-aligned with the X-ray telescopes, on XMM-Newton. The OM uses a Ritchey-Chrétien telescope design modified by field flattening optics built into the detector window (Mason et al. 2001). The OM field of view is $17 \times 17$ arcmin centred on the centre of the X-ray field of view. It has a 30 cm diameter primary mirror with a focal ratio of $f/2$ and feeds a hyperboloid secondary mirror, which modifies the focal ratio to 12.7 (focal length of about 3.8 m). From the secondary mirror, the incoming light is reflected onto a $45^\circ$ flat mirror located behind the primary, which can be rotated to direct the beam to one of two redundant filter wheel/detector assemblies. The OM telescope has a microchannel-plate intensified CCD detector (Fordham et al. 1992) in its focal plane. Figure 4.7 shows a schematic diagram of the OM telescope. An active area of $256 \times 256$ CCD pixels is used, and incoming photon events are centroided to 1/8th of a CCD pixel to yield $2048 \times 2048$ pixels on the sky, each $0.4765 \times 0.4765$ arcsec$^2$ (Mason et al. 2001).

The filter wheel has 11 apertures, one of which is blanked off to serve as a shutter, preventing light from reaching the detector (Mason et al. 2001). Another 7 filter locations house lenticular filters, 6 of which are broad-band filters (V, B, U, UVW1, UVM2, UVW2) for colour discrimination in the optical and UV bands. The
4.2 XMM-Newton data reduction

All the XMM-Newton data used in this thesis, for the study of the Seyfert galaxies NGC 3516, Mrk 509 and ESO 113-G010, were extracted in Observation Data Files (ODF) format from the XMM-Newton Science Archive (XSA)†. The ODF files were then processed with the latest version of the SAS software at the time of the analysis of each object; therefore, different SAS versions have been used for processing the data of each object. For NGC 3516, version 7.2 was used throughout the analysis, except for the production of the EPIC-pn lightcurves at a later stage using the

† http://xmm.esac.esa.int/xsa

Fig. 4.8: The current effective area curves for the OM filters. The throughput for the OM filters is folded with the detector sensitivity. Figure taken from XMM-Newton XMM-Newton OM Calibration Status (2011).

seventh filter is a white-light filter which transmits light over the full waveband of the detector. The filter effective area curves are displayed in Fig. 4.8. In addition to the broadband filters, the OM filter wheel contains an optical and a UV grism, effectively a grating-prism combination for low resolution spectroscopy. The remaining filter wheel position holds a ×4 field expander (magnifier lens) to provide high spatial resolution of the central portion of the field of view in the 3800–6500 Å band.

4.2 XMM-Newton data reduction

All the XMM-Newton data used in this thesis, for the study of the Seyfert galaxies NGC 3516, Mrk 509 and ESO 113-G010, were extracted in Observation Data Files (ODF) format from the XMM-Newton Science Archive (XSA)†. The ODF files were then processed with the latest version of the SAS software at the time of the analysis of each object; therefore, different SAS versions have been used for processing the data of each object. For NGC 3516, version 7.2 was used throughout the analysis, except for the production of the EPIC-pn lightcurves at a later stage using the

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4.2. XMM-Newton data reduction

The spectral analysis and modelling, presented in this thesis, were done using the spex\footnote{http://www.sron.nl/spex} package (Kaastra et al. 1996). For NGC 3516 version 2.01.02, for Mrk 509 version 2.01.05 and for ESO 113-G010 version 2.02.04 of spex were used at the time of the analysis. Note all the spectra shown in this thesis are background-subtracted and are in the observed frame, unless otherwise stated in the text. The adopted cosmological parameters in this thesis are \( H_0 = 73 \text{ km s}^{-1} \text{ Mpc}^{-1}, \Omega_\Lambda = 0.73 \) and \( \Omega_m = 0.27 \).

4.2.1 RGS

The RGS instruments were operated in the standard Spectro+Q mode for all the observations. Good Time Intervals (GTIs) were constructed to filter out intervals with background count rates \( > 0.4 \text{ ct s}^{-1} \) for NGC 3516 and \( > 0.1 \text{ ct s}^{-1} \) for ESO 113-G010 in CCD number 9, which is the closest to the optical axis of the telescope and therefore the most affected by background flares. For ESO 113-G010 about 8 ks was removed, leaving a net exposure time of about 95 ks for each RGS instrument. No filtering due to background flares was needed for Mrk 509, as the background was very low \( (< 0.1 \text{ ct s}^{-1}) \) and stable for the full duration of our campaign. The data were processed through the rgsproc pipeline task; the source and background first and second order spectra of RGS1 and RGS2 were extracted and the response matrices were generated. For ESO 113-G010, using the rgscombine task, we combined the RGS1 and RGS2 first-order spectra and response matrices in order to achieve better signal-to-noise for the purpose of spectral fitting. For NGC 3516, the high signal-to-noise RGS1 and RGS2 spectra were not combined and instead were fitted simultaneously together with the EPIC-pn spectra. The 6–38 Å (0.33–2.07 keV) part of the first-order RGS spectra have been used for modelling in this thesis; the data were binned by a factor of 3 (this corresponds to an average bin size of 0.04 Å, which still over-samples the RGS resolution element of \( \sim 0.07 \text{ Å FWHM} \)) in order to improve statistics.

I note here that the RGS data reduction for Mrk 509, which is not part of
this thesis, has been performed at a more advanced level than the standard SAS pipelines. The main reasons for this are the use of the RGS multi-pointing mode during the observations and the high statistical quality of the data. Full details of the data reduction of the Mrk 509 RGS data are given in Kaastra et al. (2011b).

### 4.2.2 EPIC-pn

During the *XMM-Newton* observations reported in this thesis, the EPIC-pn camera was operated in the Small-Window mode with the thin-filter for NGC 3516 and Mrk 509, and operated in the Full-Frame mode with the medium-filter for ESO 113-G010. Periods of high flaring background were filtered out before extracting scientific products. This was done by extracting a single event, high energy ($10 < E < 12$ keV) light curve, in order to create a set of GTIs for use in conjunction with the internal GTI tables, to exclude intervals of flaring particle background with count rates exceeding $0.4 \text{ ct s}^{-1}$. The GTIs were then applied to the production of the EPIC-pn spectra. The final cleaned exposure times are shown in Tables 5.1 (NGC 3516), 6.1 (Mrk 509) and 7.1 (ESO 113-G010).

The spectra and lightcurves of EPIC-pn were extracted from a circular region centred on the source. The radius of the extraction region was 40″ for NGC 3516 and Mrk 509, and 35″ for ESO 113-G010. The background was extracted from a nearby source-free region of the same size on the same CCD chip. The EPIC-pn showed no evidence of pile-up for all the observations, thus single and double events were selected. The EPIC-pn lightcurves were background-subtracted and corrected (using the *epiclccorr* SAS task) for various effects on the detection efficiency such as vignetting, bad pixels, chip gaps, Point Spread Function (PSF) variation and quantum efficiency; the task also makes corrections for quantities which vary with time and thus affect the stability of the detection, like dead time and GTIs. Response matrices were generated for each source spectrum using the SAS tasks *arfgen* and *rmfgen*.

### 4.2.3 OM broad-band filters

For the *XMM-Newton* observations of NGC 3516, the OM was operated in Image+Fast mode in all the observations, as well as in Science User Defined mode in the last two exposures of Obs. 1, Obs. 3 and Obs. 4. The images in all four observations of NGC 3516 were taken with the *U* filter; the FWHM of the source is
4.2. XMM-Newton data reduction

about 1.6″, which is consistent with the OM on-board PSF FWHM of 1.55″ in the $U$ filter. For Mrk 509, the OM was operated in Image+Fast mode for the duration of the campaign, taking data with the $V$, $B$, $U$, $UVW1$, $UVM2$ and $UVW2$ filters. A spectrum with the OM optical grism was also obtained for each Mrk 509 observation (see Sect. 4.2.4 for the data reduction of the optical grism). For ESO 113-G010, the OM was operated in Full Frame mode, as well as Science User Defined mode in the last exposure of the observation; the data were taken with the $U$, $UVW1$, $UVM2$ and $UVW2$ filters. The OM exposure times for each object are given in Tables 5.1, 6.1 and 7.1. The OM image data were processed with the SAS omichain pipeline. I performed aperture photometry on each image in an interactive way using the omsource program. Source and background regions were selected to extract the count rates, and all the necessary corrections were applied, i.e. for the point spread function (PSF) and coincidence losses, including time-dependent sensitivity (TDS) corrections. The OM count rates were extracted from a circle centred on the source nucleus. The radius of the extraction circle was 8 pixels (3.8″) for NGC 3516 and 12 pixels (5.7″) for Mrk 509 and ESO 113-G010. The background was extracted from a source-free region of the same radius.

4.2.4 OM optical grism

Mrk 509 has been observed with the OM optical grism ($V_{\text{grism}}$) during each one of the 10 XMM-Newton observations of the campaign. The images from the optical grism were first processed with the SAS omgchain pipeline (for an overview of the OM instrument see Mason et al. 2001). All the necessary corrections, including that for Modulo-8 fixed pattern noise and removal of scattered light features, were applied to obtain undistorted and rotated grism images. I then used the omgsource program to interactively identify the zero and first dispersion order spectra of our source, to properly define the source and background extraction regions and extract the calibrated spectrum from the grism images of each observation. The wavelength scales are provided as a function of the distance in pixels (at full resolution) from the centroid of the zeroth order in the extracted spectrum (see XMM-Newton OM Calibration Status (2011) for more details).

Figure 4.9 shows an example image of OM optical grism dispersion spectra of sources in the field of view, obtained in a single window mode around the target spectrum (Mrk 509). The exposure time is 5 ks. For each source in the field of
Fig. 4.9: An image of the OM optical grism dispersion spectra of sources in the field of view, obtained in a single window mode around the target spectrum (Mrk 509). The zero-order and first-order dispersion spectra of Mrk 509, including the location of the Hα line, are indicated. The image is rotated to have the dispersion direction aligned with the image columns. The exposure time is 5 ks.
4.2. XMM-Newton data reduction

Fig. 4.10: The effective area of the OM optical and UV grisms. The optical grism effective area includes my extension of the flux calibration from 6000 Å to nearly 7000 Å.

view, the grism gives dispersion spectra (i.e. the zero-order and first-order spectra) displaced from one another in the dispersion direction. The zero-order and first-order spectra of Mrk 509 are indicated. The flux calibration by default is performed between 3000 and 6000 Å for the optical grism in the SAS software. However, because the Hα λ6563 emission line appears right at the long wavelength end of the first order spectrum (see Fig. 4.9) for which no standard calibration exists, I extended the flux calibration to around 7000 Å in order to include this emission line in our spectra. The contamination by one end of the second order spectrum (which overlaps the first order one at the location of the Hα in the image) is found to be negligible compared with the strong emission from the line.

I used multiple OM spectra of the standard spectroscopic stars GD153 and HZ2 to extend the calibration by normalising them to HST spectra taken from the calspec\textsuperscript{\dag} database. This allows us to determine the inverse sensitivity function (ISF) as a function of wavelength \(\lambda\), which converts the OM count rate \(S(\lambda)\) into

\textsuperscript{\dag}http://www.stsci.edu/hst/observatory/cdbs/calspec.html
Table 4.1: The effective wavelength $\lambda_{\text{eff}}$ for each of the OM and UVOT filters. See XMM-Newton OM Calibration Status [2011] and Poole et al. [2008] for details.

<table>
<thead>
<tr>
<th>Filter</th>
<th>$\lambda_{\text{eff}}$ (Å)</th>
<th>OM</th>
<th>UVOT</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V$</td>
<td>5430</td>
<td>5402</td>
<td></td>
</tr>
<tr>
<td>$B$</td>
<td>4500</td>
<td>4329</td>
<td></td>
</tr>
<tr>
<td>$U$</td>
<td>3440</td>
<td>3501</td>
<td></td>
</tr>
<tr>
<td>$UVW1$</td>
<td>2910</td>
<td>2634</td>
<td></td>
</tr>
<tr>
<td>$UVM2$</td>
<td>2310</td>
<td>2231</td>
<td></td>
</tr>
<tr>
<td>$UVW2$</td>
<td>2120</td>
<td>2030</td>
<td></td>
</tr>
</tbody>
</table>

flux $F(\lambda)$,

$$F(\lambda) = \text{ISF}(\lambda) \times S(\lambda) \quad (4.3)$$

$S(\lambda)$ is in units of count s$^{-1}$ and $F(\lambda)$ in erg cm$^{-2}$ s$^{-1}$ Å$^{-1}$, thus ISF(\lambda) is in units of erg cm$^{-2}$ Å$^{-1}$ count$^{-1}$. The ISF in the form of effective area (in units of cm$^2$) is shown in Fig. 4.10.

4.3 Other instruments data reduction

4.3.1 Swift/XRT

For the Swift’s X-ray Telescope (XRT) data reduction of Mrk 509, I used the online Swift-XRT data products generator facility with the default settings (details given in Evans et al. 2009) to produce the X-ray spectra.

4.3.2 Swift/UVOT

The Swift’s UV/Optical Telescope (UVOT) data of Mrk 509 from Image-mode operations were taken with six broad-band filters: $V$, $B$, $U$, $UVW1$, $UVM2$ and $UVW2$. I used the uvotsource tool to perform photometry using the recommended circular aperture radius of 10 pixels ($5.0''$) and applying the standard instrumental corrections and calibration according to Poole et al. [2008]. For the purpose of spectral fitting with the spex code, I used the filter count rates and the corresponding response matrices, which were constructed using the effective area of the instrument for each of the filters.

The effective wavelengths of the OM and UVOT broad-band filters are slightly
4.3. Other instruments data reduction

different for the two instruments and are given in Table 4.1.

4.3.3 HST/COS and FUSE

The data reduction procedures of Hubble Space Telescope (HST) Cosmic Origin Spectrograph (COS) and Far Ultraviolet Spectroscopic Explorer (FUSE) data of Mrk 509 were carried out and reported by Kriss et al. (2011). The COS data processing pipeline uses a sensitivity function and the FUSE pipeline uses effective area curves to produce flux-calibrated spectra. Therefore for the purpose of fitting the UV spectra and the optical filter data together within the SPEX package, I converted the UV fluxes back to counts per second by transforming to photon units and then multiplying by the effective area integrated over the narrow bandpasses given in Table 6.4.
Chapter 5

NGC 3516: ionised outflows and X-ray variability

This chapter is based on Mehdipour et al. (2010), A&A, 514, A100.

In this chapter I present a new analysis of the soft and medium energy X-ray spectrum of the Seyfert 1 galaxy NGC 3516 obtained with the XMM-Newton RGS and EPIC instruments. Four observations, made in October 2006 and separated by a couple of days, are analysed, to investigate whether the observed variability is due to changes in the warm absorber and/or is intrinsic to the source emission. It has previously been suggested by Turner et al. (2008), who analysed the EPIC data, that the passage of a cloud, part of a disc wind, in front of the source (producing a change in the covering fraction) was the cause of a significant dip in the lightcurve during one of the observations. Using high-resolution X-ray spectroscopy with the RGS to study the warm absorber, I find that variation in the covering fraction of the absorber cannot be solely responsible for this. From simultaneous modelling of the EPIC and RGS data, it is shown that intrinsic change in the source continuum plays a much more significant role in explaining the observed flux and spectral variability than originally thought.

5.1 Introduction

The source NGC 3516 is a Seyfert 1.5 SB0 galaxy at a redshift of 0.008836 (Keel 1996) in the constellation of Ursa Major. Even from early X-ray observations of this object, signatures of a multi-phase warm absorber have been evident. From simulta-
neous far-UV and ASCA X-ray observations in 1995, a warm absorber with at least two absorption components was reported by Kriss et al. (1996). The two components differ by a factor of 8 in the ionisation parameter; the more highly ionised has a column density twice as large as the less ionised component. Netzer et al. (2002) investigated spectral variations of NGC 3516 over a period of seven years, by using archival ASCA and early Chandra observations. They reported a large drop in flux (factor of \( \sim 50 \) at 1 keV) between an ASCA observation in 1994 and the Chandra observation in 2000. Netzer et al. (2002) concluded that the variations in the observed flux and spectra at these epochs were consistent with a constant column density of line-of-sight material reacting to changes in the ionising continuum.

The galaxy NGC 3516 was observed twice by XMM-Newton in April and November 2001; both observations were partially overlapping with Chandra observations. Turner et al. (2002) presented results from the simultaneous Chandra HETGS and XMM-Newton observations made in November 2001: analysis of the Fe Kα regime showed evidence of several narrow emission features and of rapid evolution of the Fe Kα line during the observation. From a later analysis of both April and November 2001 observations, Turner et al. (2005) reported three distinct zones (phases) of gas with different ionisation parameters covering the active nucleus. The warm absorber phases found in Turner et al. (2005) are a low-ionisation UV/X-ray absorber with \( \log \xi \sim -0.5 \) and hydrogen column density of \( N_H \sim 0.5 \times 10^{22} \text{ cm}^{-2} \); a more highly ionised gas with \( \log \xi \sim 3.0 \) and \( N_H \sim 2 \times 10^{22} \text{ cm}^{-2} \) outflowing at a velocity of \( \sim 1100 \text{ km s}^{-1} \); and a phase with \( \log \xi \sim 2.5 \) and a large hydrogen column density of \( N_H \sim 25 \times 10^{22} \text{ cm}^{-2} \) covering \( \sim 50\% \) of the continuum. Turner et al. (2005) found the spectral variability in the 2001 observations to be consistent with the ionisation-state of the absorbing gas layers responding to the continuum flux variation.

More recently, four observations of NGC 3516 were performed by XMM-Newton in October 2006, interwoven with Chandra observations. The analysis of the EPIC-pn and Chandra HETGS data is published in Turner et al. (2008). They discovered a previously unknown ionisation phase in the Fe Kα regime, with \( \log \xi \sim 4.3 \) and \( N_H \sim 26 \times 10^{22} \text{ cm}^{-2} \). In line with the results from the 2001 observations, a phase with a covering fraction of \( \sim 50\% \) was confirmed. This phase was found to have \( \log \xi \sim 2.2 \) and \( N_H \sim 20 \times 10^{22} \text{ cm}^{-2} \). The source showed significant
Table 5.1: The XMM-Newton observations details of NGC 3516.

<table>
<thead>
<tr>
<th>Obs. ID</th>
<th>yyyy-mm-dd</th>
<th>hh:mm:ss</th>
<th>OM exposure (ks)</th>
<th>X-ray exposure (ks) *</th>
<th>EPIC-pn</th>
<th>RGS</th>
</tr>
</thead>
<tbody>
<tr>
<td>04012010401</td>
<td>2006-10-06</td>
<td>20:07:26</td>
<td>41.5</td>
<td>36.2</td>
<td>51.2</td>
<td></td>
</tr>
<tr>
<td>04012010501</td>
<td>2006-10-08</td>
<td>15:48:26</td>
<td>54.1</td>
<td>45.0</td>
<td>63.8</td>
<td></td>
</tr>
<tr>
<td>04012010601</td>
<td>2006-10-10</td>
<td>15:44:35</td>
<td>43.4</td>
<td>46.8</td>
<td>64.8</td>
<td></td>
</tr>
<tr>
<td>04012011001</td>
<td>2006-10-12</td>
<td>15:39:12</td>
<td>49.0</td>
<td>38.8</td>
<td>51.1</td>
<td></td>
</tr>
</tbody>
</table>

*Final cleaned X-ray exposure times are shown.

flux variability between observations, especially a dip in the lightcurve of the third observation. Turner et al. (2008) concluded that changes in the covering fraction of the phase partially covering the continuum provide a simple explanation of the dip in the lightcurve. They interpreted this as an eclipse of the continuum due to passage of a cloud across the line of sight over a period of half a day.

As part of this thesis, a new analysis of the four XMM-Newton observations of October 2006 is presented, with the emphasis put on the RGS spectra. Some details of the XMM-Newton observations of NGC 3516 are shown in Table 5.1 Sect. 5.2 focuses on the lightcurves; the spectral modelling is described in detail in Sects. 5.3 and 5.4; my findings are discussed in Sect. 5.5 and conclusions and implications of this work are presented in Chapter 8 (Sect. 8.1). All the parameter errors quoted in this chapter for NGC 3516 correspond to a $\Delta \chi^2$ of 2 for one interesting parameter.

5.2 X-ray and UV lightcurves

Figure 5.1 shows the OM (UV, top) and EPIC-pn (X-ray) lightcurves of the four observations. The source shows significant X-ray flux variability during the observations, notably the flare in Obs. 1 and the dip in Obs. 3. From visual inspection of the X-ray lightcurves, the variations in the 0.2–2.0 keV (soft X-ray) and 2.0–10.0 keV (hard X-ray) bands follow each other closely; however in Obs. 3 the ratio of soft to hard X-ray count rates clearly increases as the observation progresses, which indicates spectral variability; some evidence for a softer spectrum when brighter is also present in Obs. 1 and Obs. 4.

In contrast to the X-ray, the UV lightcurve shows no significant flaring in Obs. 1 and there is no significant dip in the UV flux in Obs. 3; it is not unusual to
5.2. X-ray and UV lightcurves

Fig. 5.1: Upper panel: Top lightcurves: the OM background-subtracted $U$ band (3000–3900 Å) lightcurves of Obs. 1 (red), Obs. 2 (purple), Obs. 3 (black) and Obs. 4 (blue); each count rate is scaled down by a factor of 4 for clarity of display and corresponds to an OM exposure of 1400 s. Middle lightcurves: the EPIC-pn background-subtracted lightcurves of the four observations in 200 s time bins over 0.2–2.0 keV. Bottom lightcurves: the EPIC-pn background-subtracted lightcurves of the four observations in 200 s time bins over 2.0–10.0 keV. Lower panel (green): the ratio of 0.2–2.0 keV (soft X-ray) to 2.0–10.0 keV (hard X-ray) lightcurves.
5.3 Preliminary modelling of the X-ray continuum and Fe Kα line

Figure 5.2 depicts an overview of the EPIC-pn and RGS spectra of the four observations: while Obs. 2 and 4 display very similar spectra (so much so that they are practically indistinguishable), that of Obs. 1 lies slightly above them, and that of Obs. 3 is clearly much fainter than all the others. The features of the spectra, in particular during the dip in Obs. 3, are discussed in the sections below.

The modelling of the 4.0–10.0 keV EPIC-pn spectrum of Obs. 2 (which is the longest of the four observations) was started by using a simple power-law (pow in spex) over the range 4.0–10.0 keV, redshifted to $z = 0.00836$. The transmission of the Galactic neutral absorption was included by applying the hot model (introduced in Sect. 3.4) in spex. The Galactic H\textsc{i} column density in our line of sight was fixed...
5.3. Preliminary modelling of the X-ray continuum and Fe Kα line

Fig. 5.3: Observation 2 EPIC-pn power-law fit (including the Gaussian Fe Kα line and Galactic absorption) over the 4.0–10.0 keV range. The fit is extrapolated to lower energies, displaying the presence of a soft excess and additional absorption in the 0.6–2.5 keV range.

to $N_H = 3.45 \times 10^{20}$ cm$^{-2}$ ([Kalberla et al. 2005]) and the gas temperature to 0.5 eV to mimic a neutral gas in collisional ionisation equilibrium. The prominent Fe Kα emission line at $\sim 6.4$ keV was modelled by a simple Gaussian profile (gaus model in spex) with its width left free to vary. The parameters obtained from the preliminary modelling of the continuum and Fe Kα line are shown in Table 5.2. Interestingly, one finds that whereas the power-law flux falls significantly in Obs. 3, that of the Fe Kα emission line remains unchanged compared to the other observations.

Figure 5.3 shows the 4.0–10.0 keV EPIC-pn fit, extrapolated to lower energies, displaying the presence of a soft excess and additional absorption in the 0.6–2.5 keV band. The latter is most likely due to the warm absorber and will be modelled in the next section, by fitting the RGS and EPIC-pn data simultaneously.

To include modelling of the soft excess, the EPIC-pn spectrum of Obs. 2 over the 0.2–10.0 keV energy range was refitted. It is found that a single power-law continuum model cannot fit the spectrum at all; a reduced chi-squared ($\chi^2$) value of 143 is obtained for 1111 degrees of freedom (d.o.f.). A modified blackbody component (mbb) was then added to the continuum in addition to the power-law.
Table 5.2: Power-law and Fe Kα emission line parameters, obtained from preliminary EPIC-pn fits (including the Galactic absorption) of all four observations over the 4.0–10 keV energy range.

<table>
<thead>
<tr>
<th>Obs.</th>
<th>Photon Index (Γ)</th>
<th>Normalisation $^a$</th>
<th>$E_0^b$</th>
<th>$E^c$</th>
<th>Flow $v^d$</th>
<th>FWHM $^e$</th>
<th>$\sigma_v^f$</th>
<th>Normalisation $^g$</th>
<th>$\chi^2_v$ / d.o.f.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.85 ± 0.02</td>
<td>2.9 ± 0.1</td>
<td>6.39</td>
<td>6.37 ± 0.02</td>
<td>+900$^{+1000}_{-900}$</td>
<td>280 ± 70</td>
<td>6000 ± 2000</td>
<td>1.1 ± 0.1</td>
<td>1.54/330</td>
</tr>
<tr>
<td>2</td>
<td>1.82 ± 0.02</td>
<td>2.5 ± 0.1</td>
<td>6.39</td>
<td>6.38 ± 0.01</td>
<td>+500$^{+400}_{-500}$</td>
<td>290 ± 40</td>
<td>6000 ± 1000</td>
<td>1.3 ± 0.1</td>
<td>1.42/361</td>
</tr>
<tr>
<td>3</td>
<td>1.75 ± 0.02</td>
<td>1.9 ± 0.1</td>
<td>6.39</td>
<td>6.38 ± 0.01</td>
<td>+500$^{+400}_{-500}$</td>
<td>290 ± 40</td>
<td>6000 ± 1000</td>
<td>1.3 ± 0.1</td>
<td>1.58/324</td>
</tr>
<tr>
<td>4</td>
<td>1.84 ± 0.02</td>
<td>2.6 ± 0.1</td>
<td>6.39</td>
<td>6.40 ± 0.01</td>
<td>$-500^{+500}_{-400}$</td>
<td>260 ± 40</td>
<td>5000 ± 1000</td>
<td>1.2 ± 0.1</td>
<td>1.38/311</td>
</tr>
</tbody>
</table>

$^a$ $10^{51}$ photons s$^{-1}$ keV$^{-1}$ at 1 keV.
$^b$ Theoretical rest frame wavelength in keV.
$^c$ Wavelength in the rest frame of NGC 3516 in keV.
$^d$ km s$^{-1}$.
$^e$ eV.
$^f$ RMS velocity in km s$^{-1}$ ($\sigma_v = \text{FWHM}/\sqrt{\ln 256}$).
$^g$ $10^{49}$ photons s$^{-1}$.
5.4. Spectral modelling of the warm absorber

The \texttt{mbb} model (Kaastra and Bari 1989) describes the spectrum of a blackbody modified by coherent Compton scattering, and is often used as a fitting device for the soft excess and the underlying soft X-ray continuum. The addition of the \texttt{mbb} component ($kT = 128$ eV) caused the $\chi^2_\nu$ to fall from 143 (1111 d.o.f.) to 21.0 (1109 d.o.f.). This is not yet a satisfactory fit, which shows the need for further modelling of the absorption in the 0.6–2.5 keV range (i.e. the warm absorber); this is discussed in the following section.

5.4 Spectral modelling of the warm absorber

In the following subsections the process of fitting the spectra with a model including warm absorption is described. I start by fitting in detail the spectrum of Obs. 2, which represents an “average” state of the source. In Sect. 5.4.1 only the RGS spectrum of Obs. 2 is fitted and in Sect. 5.4.2 both the RGS and EPIC-pn are fitted simultaneously; I then proceed to fit the spectra of all the other observations.

5.4.1 Spectral fit using a thin slab absorption model

The analysis of the warm absorber began by identifying and characterising the main absorption lines in the RGS spectrum of Obs. 2, shown in Fig. 5.4. I started by adding a \texttt{slab} component (see Sect. 3.4) to the best-fit continuum model obtained from the EPIC-pn. All the continuum parameters except the power-law photon index were left free. The photon index was let free only after an overall good fit was obtained. This helps prevent being caught in false $\chi^2_\nu$ minima and obtaining a photon index incompatible with the EPIC-pn during the $\chi^2_\nu$ minimisation. This method of fixing the power-law photon index until close to the end of the fitting is also used in Steenbrugge et al. (2003a).

Initially all the ions in the \texttt{slab} component have negligible column densities. The column density of each ion was fitted one by one, starting from the ions responsible for the strongest absorption lines in the spectrum. All the ions in a \texttt{slab} component have the same flow and RMS (broadening) velocities. So after fitting the column densities of all the ions, the velocities of some of the ions were decoupled by creating a separate \texttt{slab} component for each ion. Table 5.3 shows the velocities determined for these ions. Decoupling the velocities of only those ions with strong absorption lines improves the fit. Decoupling velocities of the ions with weak lines does not improve the fit because large errors are associated with these ions.
5.4. Spectral modelling of the warm absorber

Fig. 5.4: RGS spectrum of Obs. 2, fitted using the *slab* model described in Sect. 5.4.1. Some of the strongest absorption features are labelled.

Table 5.3: Flow and RMS (broadening) velocities of the ions with the strongest absorption lines in the Obs. 2 RGS spectrum, determined from the *slab* model best-fit.

<table>
<thead>
<tr>
<th>Ion</th>
<th>Flow $v^a$</th>
<th>RMS $v^a$</th>
<th>Observed Transitions</th>
</tr>
</thead>
<tbody>
<tr>
<td>C\textsc{vi}</td>
<td>$-800 \pm 100$</td>
<td>$300 \pm 100$</td>
<td>Ly-$\alpha$, Ly-$\beta$, Ly-$\gamma$</td>
</tr>
<tr>
<td>N\textsc{vi}</td>
<td>$-700 \pm 300$</td>
<td>$600 \pm 200$</td>
<td>He-$\alpha$, He-$\beta$, He-$\gamma$</td>
</tr>
<tr>
<td>N\textsc{vii}</td>
<td>$-800 \pm 300$</td>
<td>$900 \pm 300$</td>
<td>Ly-$\alpha$, Ly-$\beta$, Ly-$\gamma$</td>
</tr>
<tr>
<td>O\textsc{vii}</td>
<td>$-900 \pm 100$</td>
<td>$300 \pm 100$</td>
<td>He-$\alpha$, He-$\beta$, He-$\gamma$, He-$\delta$</td>
</tr>
<tr>
<td>O\textsc{viii}</td>
<td>$-1000 \pm 100$</td>
<td>$370 \pm 40$</td>
<td>Ly-$\alpha$, Ly-$\beta$, Ly-$\gamma$, Ly-$\delta$</td>
</tr>
</tbody>
</table>

$^a$km s$^{-1}$. 
5.4. Spectral modelling of the warm absorber

The ions with weak lines, which do not appear in Table 5.3, are modelled as one slab component with an outflow velocity of $900 \pm 100 \text{ km s}^{-1}$ and RMS velocity of $900 \pm 100 \text{ km s}^{-1}$.

The slab model was used only to get some understanding of the scale of velocity and column density of the ions, especially those with the clearest absorption lines in the RGS spectrum (e.g. O viii). To analyse the warm absorber in detail, the realistic xabs photoionisation model (see Sect. 3.4) was used, as described in the following subsection.

5.4.2 Spectral fit using a photoionised absorption model

I used the default xabs model in SPEX, in which the ionisation balance calculations (described in Sect. 3.1) were done using the CLOUDY (Ferland et al. 1998) code with the SED (displayed in Fig. 5.5) based on that of NGC 5548, as used in Steenbrugge et al. (2005b). This is a good approximation for NGC 3516 because both Seyfert 1.5 AGN have very similar SEDs, as shown in the NASA/IPAC Extragalactic Database (NED). The advantage of the xabs photoionisation model over the slab model is that all relevant ions are taken into account, including those that would be detected only with marginal significance or not detected at all with the slab model (Kaastra et al. 2012a).

I started with the EPIC-pn best-fit continuum and Fe Kα model established in Sect. 5.3, leaving the power-law, mbb and Fe Kα parameters free (except for the power-law photon index, which was kept fixed to the value given in Table 5.2 until close to the end of the fitting procedure). The xabs model was applied to the continuum to fit the ionisation parameter ($\xi$), the hydrogen column density ($N_H$), the flow and RMS velocities in the EPIC-pn and RGS spectra of Obs. 2 simultaneously. The elemental abundances were fixed at the proto-solar values of Lodders (2003). Because EPIC-pn, RGS1 and RGS2 spectra were being fitted simultaneously, the relative normalisations of the instruments were allowed to be free parameters. The instrumental normalisation of RGS1 was fixed to 1 and the normalisations of the RGS2 and EPIC-pn were freed. This way problems with differences in relative normalisations between different instruments are avoided (Bhustin et al. 2003). The EPIC-pn spectrum helps to establish the underlying 0.2–10 keV continuum level, however, since the number of RGS bins containing the spectral features is much smaller than the higher signal-to-noise EPIC-pn bins, care should be taken when si-
multaneously fitting EPIC-pn CCD and RGS grating spectra. One cannot just rely on the goodness of the $\chi^2$ fit and it is important to check all the spectral features in RGS1 and RGS2 have been fitted well and are consistent with atomic transitions.

One $x_{\text{abs}}$ component was then included in the model. This corresponds to phase B in Table 5.4, where the phases are sorted by increasing value of $\xi$. Adding the first $x_{\text{abs}}$ component improved $\chi^2_\nu$ from 25.3 (2801 d.o.f.) to 3.91 (2797 d.o.f.), by fitting $\xi$, $N_{\text{H}}$, flow and RMS velocities. The model still required more absorption at $\sim11$–$15$ Å (expected to be due to hot iron, Fe$_{\text{XVII}}$–Fe$_{\text{XXIV}}$) and $\sim16$–$17$ Å (most likely due to cold iron, Fe$_{\text{I}}$–Fe$_{\text{XIV}}$). To produce a better fit to the data, a second $x_{\text{abs}}$ component was accordingly introduced to the model. This corresponds to phase C in Table 5.4. The addition of phase C, which is the one with the highest ionisation parameter, further improved $\chi^2_\nu$ from 3.91 (2797 d.o.f.) to 1.88 (2793 d.o.f.). It was found that after adding two $x_{\text{abs}}$ components, absorption by iron, especially the M-shell iron (Fe$_{\text{I}}$–Fe$_{\text{XIV}}$) forming the Unresolved Transition Array (UTA) at $\sim16$–$17$ Å (Behar et al. 2001), was still not properly modelled. To model the UTA, a phase with an ionisation lower than the two previously identified was required. Therefore, a third $x_{\text{abs}}$ component (phase A) was added to the model. The addition of phase A improved $\chi^2_\nu$ from 1.88 (2793 d.o.f.) to 1.63 (2789 d.o.f.)
as the UTA was fitted well. At this point, the power-law photon index ($\Gamma$) was left free to vary in the fitting procedure for Obs. 2, but neither the value of $\Gamma$ (1.82) nor $\chi^2_\nu$ changed significantly.

To attempt to further improve the quality of the fit, the abundances of only those elements with the strongest absorption features in the RGS spectrum were freed: N, O and Fe. In order not to increase the number of free parameters unnecessarily, the abundances of all three phases were coupled. The precise abundances of elements in each phase cannot be accurately determined, because letting them all free results in some cases in unphysical values. Assuming that different phases have the same abundances is already a more progressive approach than the alternative of assuming cosmic abundances for all the phases. For example, the abundance coupling approach is also used in Kaastra et al. (2003), where they fixed the abundances of a cool gas component to those of a hot one to reduce the number of free parameters. Freeing the N, O and Fe abundances produced a better fit, because $\chi^2_\nu$ fell from 1.63 (2788 d.o.f.) to 1.52 (2785 d.o.f.).

One of the ionisation phases in Turner et al. (2008) with log $\xi$ of 2.2 has a partial covering fraction. Therefore, I tested at this stage of the fitting process whether any of the three phases was partially covering the source. The covering fraction in the line of sight $C_f$ (see Sect. 3.7) of the three phases was freed from the default value of 1. The $C_f$ value of one of the phases (phase B with log $\xi$ of 2.4) was found to change from 1 to 0.55, while the covering fraction of the other two phases remained practically unchanged. By freeing the covering fraction of phase B, $\chi^2_\nu$ fell from 1.52 (2785 d.o.f.) to 1.44 (2784 d.o.f.). Indeed there are absorption lines in the 11–13 Å region of the RGS spectrum, as well as the UTA and the O vii He-\(\alpha\) line that are not fitted well if $C_f$ is fixed to 1. Thus some partial covering of the continuum is necessary for phase B, but this is not the case for the other two phases. Therefore, phase B was allowed to have a free $C_f$, and the $C_f$ values of phases A and C were fixed to 1. The best-fit parameters for Obs. 2 ($x_{\text{abs}}$, abundances, power-law and mbb) are listed in Tables 5.4, 5.5 and 5.6 respectively. A plot of the whole RGS spectrum, the EPIC-pn data and the best-fit model for Obs. 2 is shown in Fig. 5.6. In Fig. 5.7 close-ups of the RGS spectrum and the best-fit model are presented.
Table 5.4: Best-fit parameters of the three-phase \textit{xabs} model for the four \textit{XMM-Newton} observations of NGC 3516, obtained from the simultaneous fitting of the EPIC-pn, RGS1 and RGS2 spectra.

<table>
<thead>
<tr>
<th>Obs.</th>
<th>Phase A: $\log \xi^a$</th>
<th>$N_H^b$</th>
<th>Flow $v^c$</th>
<th>RMS $v^c$</th>
<th>Phase B: $\log \xi^a$</th>
<th>$N_H^b$</th>
<th>Flow $v^c$</th>
<th>RMS $v^c$</th>
<th>$C_f^d$</th>
<th>Phase C: $\log \xi^a$</th>
<th>$N_H^b$</th>
<th>Flow $v^c$</th>
<th>RMS $v^c$</th>
<th>$\chi^2_v / \text{d.o.f.}^e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.95 ± 0.02</td>
<td>0.33 ± 0.01</td>
<td>−100 ± 40</td>
<td>60 ± 10</td>
<td>2.41 ± 0.04</td>
<td>1.7 ± 0.2</td>
<td>−1500 ± 100</td>
<td>500 ± 100</td>
<td>0.64 ± 0.09</td>
<td>3.00 ± 0.05</td>
<td>1.2 ± 0.2</td>
<td>−800 ± 300</td>
<td>300 ± 100</td>
<td>1.41/2746</td>
</tr>
<tr>
<td>2</td>
<td>0.96 ± 0.02</td>
<td>0.34 ± 0.01</td>
<td>−100 ± 30</td>
<td>40 ± 10</td>
<td>2.42 ± 0.04</td>
<td>2.0 ± 0.3</td>
<td>−1500 ± 100</td>
<td>500 ± 100</td>
<td>0.55 ± 0.04</td>
<td>2.99 ± 0.03</td>
<td>1.3 ± 0.2</td>
<td>−1000 ± 100</td>
<td>400 ± 100</td>
<td>1.44/2784</td>
</tr>
<tr>
<td>3</td>
<td>0.87 ± 0.02</td>
<td>0.43 ± 0.02</td>
<td>−200 ± 40</td>
<td>40 ± 10</td>
<td>2.43 ± 0.03</td>
<td>3.2 ± 0.4</td>
<td>−1600 ± 200</td>
<td>400 ± 100</td>
<td>0.64 ± 0.04</td>
<td>3.07 ± 0.04</td>
<td>1.7 ± 0.2</td>
<td>−800 ± 200</td>
<td>400 ± 100</td>
<td>1.41/2689</td>
</tr>
<tr>
<td>4</td>
<td>0.97 ± 0.02</td>
<td>0.37 ± 0.01</td>
<td>−200 ± 20</td>
<td>30 ± 10</td>
<td>2.39 ± 0.05</td>
<td>2.0 ± 0.1</td>
<td>−1500 ± 100</td>
<td>600 ± 100</td>
<td>0.54 ± 0.04</td>
<td>2.99 ± 0.02</td>
<td>1.7 ± 0.2</td>
<td>−1000 ± 100</td>
<td>500 ± 100</td>
<td>1.42/2724</td>
</tr>
</tbody>
</table>

$^a$\, erg cm s$^{-1}$.

$^b$\, 10$^{22}$ cm$^{-2}$.

$^c$\, km s$^{-1}$.

$^d$ The covering fraction in the line of sight of phase B, which is a free parameter. $C_f$ of phases A and C is fixed to 1.

$^e$ The $\chi^2_v$ values are further improved by including the modelling of the observed emission features discussed in Sect. 5.4.5.

Table 5.5: The elemental abundances of the three-phase \textit{xabs} model of NGC 3516 Obs. 2 fitted simultaneously to the EPIC-pn, RGS1 and RGS2 spectra. The abundances of the three phases were coupled to each other in the fits. All the abundances are relative to the proto-solar model of Lodders (2003). The reference element is H. The abundance of elements, other than N, O and Fe is fixed to 1.

<table>
<thead>
<tr>
<th>Element</th>
<th>Abundance relative to H</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>1.5 ± 0.1</td>
</tr>
<tr>
<td>O</td>
<td>1.4 ± 0.1</td>
</tr>
<tr>
<td>Fe</td>
<td>1.8 ± 0.1</td>
</tr>
<tr>
<td>Other elements</td>
<td>1 (f)</td>
</tr>
</tbody>
</table>
Table 5.6: Best-fit parameters of the NGC 3516 continuum, obtained from the three-phase $x_{\text{abs}}$ model simultaneous fit to the EPIC-pn, RGS1 and RGS2 spectra.

<table>
<thead>
<tr>
<th>Obs.</th>
<th>Power-law:</th>
<th>Modified blackbody:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Photon Index ($\Gamma$)</td>
<td>Normalisation $^a$</td>
</tr>
<tr>
<td>1</td>
<td>1.85 ± 0.02</td>
<td>3.3 ± 0.1</td>
</tr>
<tr>
<td>2</td>
<td>1.82 ± 0.01</td>
<td>2.8 ± 0.1</td>
</tr>
<tr>
<td>3</td>
<td>1.70 ± 0.02</td>
<td>1.9 ± 0.1</td>
</tr>
<tr>
<td>4</td>
<td>1.84 ± 0.02</td>
<td>2.9 ± 0.1</td>
</tr>
</tbody>
</table>

$a$ $10^{51}$ photons s$^{-1}$ keV$^{-1}$ at 1 keV.
$b$ eV.
$c$ Emitting area times square root of the electron density in $10^{33}$ cm$^{0.5}$.

Fig. 5.6: NGC 3516 Obs. 2 best-fit $x_{\text{abs}}$ model, fitted simultaneously to the RGS and EPIC-pn spectra. The RGS data are shown in blue, the EPIC-pn data in red and the models in black. Close-ups of the RGS spectrum, showing the spectral features more clearly, are presented in Fig. 5.7. Note that both RGS and EPIC-pn spectra in this figure have been divided by the instrument’s effective area, thus are plotted on the same scale.
Fig. 5.7: Close-ups of the NGC 3516 Obs. 2 best-fit xabs model, fitted simultaneously to the RGS and EPIC-pn spectra. The RGS data are shown in blue, the EPIC-pn data in red and the models in black. *Figure continued next page.*
5.4. Spectral modelling of the warm absorber

Fig. 5.7: Continued from previous page.
5.4. Spectral modelling of the warm absorber

Having obtained the $x_{\text{abs}}$ model best-fit for Obs. 2, I used it as the starting point for each of the other observations, leaving all the parameters quoted so far free, with the exception of the abundances of the $x_{\text{abs}}$ phases, which were fixed at the Obs. 2 best-fit (the abundance values are shown in Table 5.5). The best-fit parameters of the continuum and ionisation phases of Obs. 1, Obs. 3 and Obs. 4, modelled with the $x_{\text{abs}}$ photoionised absorption, are also shown in Tables 5.4 and 5.5. Note that the $\chi^2_\nu$ values in Table 5.4 are further improved by modelling the observed emission features discussed in Sect. 5.4.5. In the following (Sect. 5.4.3), it is described how the Obs. 2 best-fit was applied to the Obs. 3 spectrum to investigate whether the covering fraction of phase B is variable or not.

5.4.3 Spectral variability in Obs. 3

As shown in Table 5.4, phase B in Obs. 2 has a best-fit covering fraction $C_f$ of 0.55. This phase B is very similar to the partially covering phase (zone 3) of Turner et al. (2008) in terms of the ionisation parameter. I found log $\xi \sim 2.4$ versus Turner et al.’s log $\xi \sim 2.2$. The uncertainty in log $\xi$ is about ±0.1 for both cases, thus the difference between the values is not significant. However, the column density of my phase B ($N_H \sim 2.0 \times 10^{22}$ cm$^{-2}$) is about a factor of 10 smaller than that in Turner et al.’s ($N_H \sim 20 \times 10^{22}$ cm$^{-2}$). In Sect. 5.5.2, the $N_H$ values of warm absorber phases in NGC 3516 found by different authors are discussed. Turner et al. (2008) explained the dip in the X-ray lightcurve of Obs. 3 by varying only the covering fraction of their zone 3. In order to try and reproduce their results, the Obs. 2 best-fit (obtained in Sect. 5.4.2) was applied to Obs. 3 by keeping all the parameters fixed and freeing only the covering fraction. As for Obs. 2, the EPIC-pn and RGS spectra were fitted simultaneously. Applying the Obs. 2 best-fit to Obs. 3 gives an initial $\chi^2_\nu$ of 225 (2711 d.o.f.). One finds that by freeing only the covering fraction no good fit is achieved; the covering fraction goes to 1 and a $\chi^2_\nu$ of 130 (2710 d.o.f.) is obtained. On the other hand, if only the continuum parameters are freed, a much better fit is obtained, $\chi^2_\nu$ of 1.76 (2707 d.o.f.). Figures 5.8 and 5.9 depict the difference between the two approaches to Obs. 3, which proves that changing the continuum parameters is a much more feasible solution than changing only the covering fraction of phase B in order to fit the Obs. 3 spectrum.
5.4. Spectral modelling of the warm absorber

Fig. 5.8: Simultaneous fit made to the EPIC-pn and RGS spectra of NGC 3516 Obs. 3 with the best-fit model of Obs. 2 and fitting only the covering fraction $C_f$ of phase B. The $\chi^2$ is 130 (2710 d.o.f.). The RGS data are shown in blue, the EPIC-pn data in red and the models in black. 

*Figure continued next page.*
Fig. 5.8: Continued from previous page.
Fig. 5.9: Simultaneous fit made to the EPIC-pn and RGS spectra of NGC 3516 Obs. 3 with the best-fit model of Obs. 2 and fitting only the continuum parameters (maintaining $C_f = 0.55$). The $\chi^2$ is 1.76 (2707 d.o.f.). The RGS data are shown in blue, the EPIC-pn data in red and the models in black. The significance of the O\text{vii} He-$\gamma$ and Ca\text{xiv} lines is discussed in Sect. 5.4.4. Figure continued next page.
5.4. Spectral modelling of the warm absorber

Fig. 5.9: Continued from previous page.
I then tried freeing both the continuum and covering fraction. In this case, the covering fraction becomes 0.70 and $\chi^2_{\nu}$ goes to 1.65 (2706 d.o.f.). Then the ionisation parameter and $N_H$ of the three xabs phases, parameters of the Fe Kα line and the relative normalisations of the EPIC-pn and RGS instruments were freed; the $\chi^2_{\nu}$ improved to 1.42 (2695 d.o.f.). Finally, the velocities of the xabs phases were freed, keeping the abundances fixed. In this case, the fit does not improve significantly, a $\chi^2_{\nu}$ of 1.41 (2689 d.o.f.) was obtained. The best-fit results for Obs. 3 and the other three observations (as described in Sect. 5.4.2), are shown in Tables 5.4, 5.5 and 5.6.

It is worth noting the advantage of modelling both the RGS and EPIC-pn together, which leads to simultaneously constraining the broadband continuum using the EPIC-pn and modelling the absorption features with the RGS. This approach has a drawback because due to smaller statistical fractional errors associated with the EPIC-pn compared to the RGS, the best-fit favours the EPIC-pn. But by making sure that the RGS absorption features are fitted properly, this weakness is not a problem.

5.4.4 The partially covering phase B

Figure 5.10 shows how each one of the three phases in my warm absorber model contributes to the best-fit for the four observations. Phases A, B and C are plotted in black, blue and red, respectively. Phase A, which is the lowest ionisation phase, is associated with M-shell Fe absorption forming the UTA (Behar et al. 2001) between 16 and 17 Å. Phase C, the highest ionisation phase, is associated with highly ionised Fe. Phase B, of intermediate ionisation, is the phase with the partial covering fraction.

In the previous subsection (Sect. 5.4.3), it was shown that by changing only the covering fraction of phase B, one cannot fit the Obs. 3 spectrum. To confirm that $C_f$ of phase B does not change significantly between observations, I examined the model to look for absorption lines unique to phase B (i.e. that do not appear in phases A and C) and to see if they change between Obs. 2 and Obs. 3. This is important because by observing a change in the depth of these lines, one can investigate the effect of a covering fraction change. There are two such absorption lines, sufficiently detectable by the RGS, which are modelled only by phase B. They are Ovii He-γ (17.8 Å) and Ca xiv (24.1 Å). Figure 5.11 shows the Ovii He-γ
Fig. 5.10: The best-fit warm absorber xabs model for NGC 3516 showing the three phases applied separately to the continuum (phase A: black, phase B: blue, phase C: red) from simultaneous fitting of the EPIC-pn and RGS spectra of Obs. 2 (top) and Obs. 3 (bottom). The best-fit parameters of the models are given in Tables 5.4, 5.5, and 5.6. The models for Obs. 1 and Obs. 4 look very similar to that of Obs. 2 (top).
and Ca XIV lines in the model. Comparing the fits in Figs. 5.7 (Obs. 2) and 5.9 (Obs. 3), one can see that the O VII He-\(\gamma\) and Ca XIV are fitted well in both. It is important to note that in both figures the covering fraction value is the same (i.e. \(C_f = 0.55\)). If the covering fraction of phase B had changed significantly in Obs. 3, one would have expected the O VII He-\(\gamma\) and Ca XIV lines in Fig. 5.9 not to be fully fitted. The fact that they are fitted well by varying only the continuum parameters is an extra piece of evidence that the variability seen in the lightcurve is mostly intrinsic to the source, and not due to the warm absorber.

5.4.5 Narrow and broad emission features

The most significant narrow emission feature in the RGS spectra of the four observations of NGC 3516 is the O VII forbidden line at rest frame wavelength of 22.10 \(\AA\) (see Sect. 3.2.2 for triplet emission lines from He-like ions). Figure 5.12 shows the Obs. 2 and Obs. 3 spectra and best-fit around the O VII triplet region. This line was modelled with a Gaussian profile (\texttt{gaus} in SPEX), and its best-fit parameters are given in Table 5.7. The RGS spectrum of NGC 3516 around the O VII triplet is
5.4. Spectral modelling of the warm absorber

Table 5.7: The best-fit parameters of the narrow O\textsuperscript{vii} forbidden emission line detected in the RGS spectra of NGC 3516, shown in Fig. 5.12, obtained by adding a Gaussian component to the best-fit x\textsubscript{abs} model of all four observations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Obs. 1</th>
<th>Obs. 2</th>
<th>Obs. 3</th>
<th>Obs. 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_0$\textsuperscript{a}</td>
<td>22.10</td>
<td>22.10</td>
<td>22.10</td>
<td>22.10</td>
</tr>
<tr>
<td>$\lambda$\textsuperscript{b}</td>
<td>22.11 ± 0.06</td>
<td>22.09 ± 0.04</td>
<td>22.11 ± 0.02</td>
<td>22.12 ± 0.08</td>
</tr>
<tr>
<td>Flow $v$\textsuperscript{c}</td>
<td>+100 ± 800</td>
<td>−100 ± 500</td>
<td>+100 ± 300</td>
<td>+300 ± 1100</td>
</tr>
<tr>
<td>FWHM\textsuperscript{d}</td>
<td>&lt; 0.1</td>
<td>&lt; 0.1</td>
<td>&lt; 0.1</td>
<td>&lt; 0.1</td>
</tr>
<tr>
<td>$\sigma_v$\textsuperscript{e}</td>
<td>&lt; 600</td>
<td>&lt; 600</td>
<td>&lt; 600</td>
<td>&lt; 600</td>
</tr>
<tr>
<td>Line Normalisation\textsuperscript{f}</td>
<td>1.0 ± 0.6</td>
<td>1.0 ± 0.6</td>
<td>1.7 ± 0.5</td>
<td>0.9 ± 0.7</td>
</tr>
</tbody>
</table>

\textsuperscript{a} Theoretical rest frame wavelength in Å.

\textsuperscript{b} Wavelength in the rest frame of NGC 3516 in Å.

\textsuperscript{c} km s\textsuperscript{−1}.

\textsuperscript{d} Å.

\textsuperscript{e} RMS velocity in km s\textsuperscript{−1} ($\sigma_v = \text{FWHM}/\sqrt{\ln 256}$).

\textsuperscript{f} $10^{49}$ photons s\textsuperscript{−1}.

very similar to that of NGC 5548 presented by Steenbrugge et al. (2003a): in that case, the forbidden line is present in emission and outflowing at around 110 km s\textsuperscript{−1}, the intercombination line is absent or very weak and the resonance line is seen in absorption; there are also absorption lines by O\textsuperscript{v} and O\textsuperscript{vi} in both NGC 3516 and NGC 5548. As suggested by Steenbrugge et al. (2003a), one possible explanation for not detecting O\textsuperscript{vii} intercombination emission is blending of the intercombination line with absorption by O\textsuperscript{vi}.

From Figs. 5.7 and 5.9 an excess of emission is noticeable in the RGS data at around 18.0 to 18.5 Å. This excess is observed in all four observations. Also, in this region of the spectrum, phase A, the lowest-ionised phase, produces absorption by O\textsuperscript{vi}. The excess emission was first fitted in Obs. 2 with a simple Gaussian profile; best-fit line wavelength of 18.16 ± 0.04 Å (in the rest frame of the AGN) and FWHM of 0.47 ± 0.09 Å ($\sigma_v = 3300 ± 600$ km s\textsuperscript{−1}) were obtained with a $\chi^2$ of 1.40 (2781 d.o.f.). The wavelength of the emission line does not correspond to any prominent transition, unless this is emission by O\textsuperscript{viii} Ly-\textalpha (rest-frame $\lambda$ of 18.97 Å) with an outflow velocity of about 13000 km s\textsuperscript{−1}. Therefore, I investigated as an alternative whether the excess could be caused by a relativistically-broadened
Fig. 5.12: Presence of forbidden O\textsuperscript{vii} line emission in the RGS spectra of NGC 3516. The RGS data are shown in blue, the EPIC-pn data in red and the models in black. Spectra from Obs. 2 are shown in the top and from Obs. 3 in the bottom panel.
5.5 Discussion

O VIII accretion disc emission line. If emission from the inner disc is influenced by general relativistic effects, the lines would appear to be broad and asymmetric. These lines were first proposed to explain the spectra of the Narrow Line Seyfert 1 galaxies MCG –6-30-15 and Mrk 766 (Branduardi-Raymont et al. 2001). A narrow emission line (delt component in spex) was added at the rest frame wavelength of the O VIII Ly-α line (18.97 Å) at the redshift of NGC 3516, and was convolved with the relativistic disc line profile of Laor (1991) (laor in spex). Parameters of the laor component are the disc inner and outer radii $r_{\text{in}}$ and $r_{\text{out}}$, its inclination angle $i$ and the emissivity index $q$, which appears in the emissivity law, taken to be proportional to $(r^2 + h^2)^{-q/2}$, where $r$ is the radius in the accretion disc and $h$ a scale height. By adding the relativistic O VIII line to the xabs best-fit model of Obs. 2, the fit improved as $\chi^2$ fell from 1.44 (2784 d.o.f., Table 5.4) to 1.40 (2779 d.o.f.) and the excess was well fitted. The line profile and the best-fit are shown in Fig. 5.13.

The inner disc radius is found to be $14 \pm 3 GM/c^2$ and the outer disc radius is poorly constrained. The signal in the red tail of the line is not strong enough to be modelled accurately; therefore, as the asymmetry of the line is not very pronounced in the data, the broadened Gaussian and the Laor profile fit the excess equally well; however, as explained earlier, a Gaussian line profile does not correspond to any prominent transition at the fitted wavelength. The disc inclination angle is constrained very well in the model for all four observations; this is because its value strongly depends on the position of the bulk of the excess emission in the spectrum: a higher inclination angle causes the emission line profile, shown in Fig. 5.13 (bottom), to move to lower energies and vice versa. As the excess emission is clearly positioned with respect to the continuum, the disc inclination angle is derived to be $33^\circ \pm 2$.

5.5 Discussion

In this chapter, the advantage of combining RGS high resolution with EPIC-pn spectroscopy in modelling an AGN warm absorber was demonstrated. EPIC-pn constrains the continuum well, but has insufficient resolution to resolve absorption and emission features seen in the warm absorber (e.g. the Fe UTA and O VIII Ly-α absorption as well as the O VII He-α (f) emission line shown in Figs. 5.7 and
5.5. Discussion

Therefore, to investigate changes in the warm absorber over time, careful examination and fitting of the RGS spectrum are needed alongside fitting the EPIC-pn spectrum. In the subsections below I discuss my results and their physical implications.

5.5.1 The Fe Kα line

The broad Fe Kα line at \( \sim 6.4 \) keV detected in the NGC 3516 spectrum was modelled with a simple Gaussian profile in the analysis presented in this chapter. For an in-depth spectral analysis of the Fe K regime in NGC 3516 the reader is referred to

**Fig. 5.13:** Top panel: the Obs. 2 best-fit \textit{xabs} model fitted simultaneously to the RGS and EPIC-pn spectra of NGC 3516 with a relativistically-broadened O \textit{viii} Ly-\( \alpha \) included (compare with Fig. 5.7 where the line is not included). The RGS data are shown in blue, the EPIC-pn data in red and the models in black. Middle panel: residuals of the fit in the top panel. Bottom panel: the Obs. 2 best-fit model of the relativistic O \textit{viii} Ly-\( \alpha \) emission line added to the continuum. The model is shown in the observed frame, and for clarity of presentation no absorption component of the model is included.
5.5. Discussion

e.g. Turner et al. (2008) in which the Chandra HETGS spectrum is used to model the Fe Kα, Fe Kβ and Fe XXVI emission lines in detail. However, from my simple modelling of the line, described in Sect. 5.3 (Table 5.2), I found that the Fe Kα flux remains practically unchanged between observations, whereas the X-ray continuum flux falls significantly in Obs. 3. It is known that the variability of the Fe Kα line in general is not correlated to that of the observed continuum in a trivial manner (e.g. Miniutti and Fabian 2004). The iron line does not always respond to variations in the continuum: in some cases the Fe Kα line appears to be constant while the continuum varies by a large amplitude (e.g. Markowitz et al. 2003). Using the EPIC-pn spectra, one cannot examine the Fe Kα profile as accurately as with the Chandra HETGS, and since the Fe Kα is not relevant to the main thrust of this work it is not discussed any further.

5.5.2 The warm absorber structure

Three phases of ionisation are found to be adequate to model the warm absorption in NGC 3516. The elemental abundances are unlikely to be different in the three phases, because it is possible to fit the spectrum very well by coupling all the abundances at values close to solar (Table 5.5). There is also no need for a large over-abundance of iron to fit the UTA.

A comparison of $\xi$, $N_H$ and outflow velocity values of warm absorber phases from recent observations of NGC 3516 reported by different authors is shown in Table 5.8. The ionisation parameters of phases B and C are remarkably similar to those found by Turner et al. (2005) during the 2001 observations. I found no need for absorption by a fourth phase (identified by Chandra HETGS to correspond to $\log \xi \sim 4.3$ in Turner et al. 2008) from my simultaneous EPIC-pn and RGS fittings, which are not very sensitive to this high ionisation gas. Note that log $\xi$ values are not strictly comparable as they are SED dependent, although the differences are likely to be only of the order of some tenth of dex. The outflow velocity of the partially covering phase B is practically the same as that in Turner et al. (2008) (their partially covering Zone 3); these phases also have very similar ionisation parameters, suggesting they represent the same photoionised gas. The second phase in Turner et al. (2005), which was also partially covering, is again very similar to my phase B in terms of ionisation parameter and outflow velocity (albeit this is smaller in 2005). The pattern that emerges by comparing the outflow velocities of all the
phases found by different authors is the existence of low-ionised phases with a very low outflow velocity and higher ionisation phases with outflow velocities between 1000 km s\(^{-1}\) and 1500 km s\(^{-1}\).

The partially covering phase is the phase with the highest outflow velocity and thus the most likely closest to the central engine. Since no changes in the occultation of the nuclear source are found in this work, there is no evidence of a transverse component of velocity for this phase. The minimum distance of this phase from the central engine can be estimated assuming the measured outflow velocity to be greater than or equal to the escape velocity \(v_{\text{esc}} = \sqrt{2GM/r}\), where \(G\) is the gravitational constant, \(M\) the black hole mass and \(r\) the distance of the absorber phase from the black hole. Since the partially covering phase B is outflowing at 1500 km s\(^{-1}\), using the NGC 3516 black hole mass estimate of \(2.95 \times 10^7\ M_\odot\) (Niko\(l\)ajuk et al. 2006), one obtains \(r \gtrsim 0.1\) pc. Using the expression for the ionisation parameter definition (Eq. 3.8) and taking \(L \approx 3.85 \times 10^{43}\) erg s\(^{-1}\) (derived from the fit of Obs. 2) one finds the hydrogen number density \(n \lesssim 1.3 \times 10^8\) cm\(^{-3}\). Combining this with the relation \(N_H \sim n\Delta r\), where \(\Delta r\) is the thickness of the absorber phase, yields \(\Delta r \gtrsim 5 \times 10^{-5}\) pc. This suggests a thin spherical shell of gas, which is a feasible scenario for partial covering.

The column densities \(N_H\) of all three phases of my warm absorber model cover a relatively small range: \(\sim 0.4-2 \times 10^{22}\) cm\(^{-2}\), and I do not find “heavy” (\(\gtrsim 20 \times 10^{22}\) cm\(^{-2}\)) absorber phases as in Turner et al. (2005, 2008), especially those corresponding to my phase B. Still my range of \(N_H\) is consistent with the values obtained from other X-ray observations of NGC 3516: Costantini et al. (2000) found a warm absorber column of \(\sim 2-3 \times 10^{22}\) cm\(^{-2}\) from BeppoSAX spectra; Netzer et al. (2002) found a line-of-sight absorber with \(N_H\) of \(\sim 1 \times 10^{22}\) cm\(^{-2}\) from both a 1994 ASCA observation and a 2000 Chandra observation; Markowitz et al. (2008) found their two warm absorber phases to have \(N_H\) of \(\sim 4\) and \(5.5 \times 10^{22}\) cm\(^{-2}\) (Table 5.8).

Turner et al. (2005) concluded that their three absorber phases cannot be in thermal equilibrium with each other in NGC 3516. To investigate this, I examined the thermal stability phase diagram (i.e. the S-curve, described in Sect. 3.3) of NGC 3516. From the ionisation balance calculations (described in Sect. 3.1) used in the default xabs model in SPEX, based on a CLOUDY (Ferland et al. 1998) run using the SED of NGC 5548 given in Steenbrugge et al. (2005b) (a good approximation
Table 5.8: Comparison of the ionisation parameters, hydrogen column densities and outflow velocities of the NGC 3516 warm absorber phases found in recent observations, shown in increasing order of $\xi$.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>log $\xi $ $^e$ ~ $N_H$ $^f$ ~ $v^g$ ~</td>
<td>log $\xi $ $^e$ ~ $N_H$ $^f$ ~ $v^g$ ~</td>
<td>log $\xi $ $^e$ ~ $N_H$ $^f$ ~ $v^g$ ~</td>
<td>log $\xi $ $^e$ ~ $N_H$ $^f$ ~ $v^g$ ~</td>
</tr>
<tr>
<td>- - -</td>
<td>- - -</td>
<td>-2.4 0.2 ? 1</td>
<td>- - - -</td>
</tr>
<tr>
<td>-0.5 0.5 -200</td>
<td>0.3 5.5 ?</td>
<td>0.25 0.05 ? 2</td>
<td>0.9 0.4 -100 A</td>
</tr>
<tr>
<td>2.5 25 -1100</td>
<td>- - -</td>
<td>2.2 20 -1600 3</td>
<td>2.4 2 -1500 B</td>
</tr>
<tr>
<td>3.0 2 -1100</td>
<td>3.7 4 -1100 $^h$</td>
<td>4.3 26 -1000 4</td>
<td>3.0 1 -900 C</td>
</tr>
</tbody>
</table>

$^a$ From the Apr. and Nov. 2001 XMM-Newton EPIC-pn spectra. The values of the ionisation parameter in $\xi$ form are given in Turner et al. (2008).

$^b$ From the Oct. 2005 Suzaku XIS and HXD spectra.

$^c$ From the Oct. 2006 XMM-Newton EPIC-pn and Chandra HETGS spectra.

$^d$ From the Oct. 2006 XMM-Newton EPIC-pn and RGS spectra.

$^e$ erg cm s$^{-1}$.

$^f$ 10$^{22}$ cm$^{-2}$.

$^g$ Flow velocity in km s$^{-1}$.

$^h$ Based on the velocity obtained in Turner et al. (2005).
5.5. Discussion

Fig. 5.14: The thermal stability phase diagram (S-curve) obtained from the CLOUDY ionisation balance calculations used in the default xabs model in SPEx. The position of the three warm absorber phases of NGC 3516 (phases A, B and C), along with their ranges of values and errors obtained from my best-fits to the four XMM-Newton observations (Table 5.4), are shown as magenta strips on the curve. Phase A is the one with the lowest $T$ and phase C the one with the highest $T$. The three warm absorber phases are not in pressure equilibrium as they are not overlapping in $\Xi$ on the S-curve.

for NGC 3516 as both Seyfert 1.5 AGN have very similar SEDs), I have obtained the corresponding S-curve, which is shown in Fig. 5.14. I find the three warm absorber phases identified in NGC 3516 in this work are unlikely to be in pressure equilibrium as their $\Xi$ values are not overlapping on the S-curve of Fig. 5.14. Since also they are outflowing with different velocities, I conclude that the three warm absorber phases in NGC 3516 are likely to be out of pressure equilibrium with each other. Because the ionisation parameters, column densities and outflow velocities of phases B and C are similar (although not in pressure equilibrium in Fig. 5.14), and more importantly the covering fraction of phase B is not variable, phase B could have the same origin as the fully covering phase C. This also disfavours a clumpy disc-wind scenario as the most likely explanation for the origin of phase B.
5.5.3 Narrow and broad emission features

The RGS spectrum shows evidence for both narrow and broad emission features. The O\textsuperscript{vii} (f) emission line is found to have a lower flow velocity compared to the observed absorption lines of the high ionisation phases B and C; the flow velocity is in fact consistent with zero and with that of the lowest ionisation phase A. Smith et al. (2008) have observed the O\textsuperscript{vii} (f) line to have a very low outflow velocity compared to other soft X-ray emission lines in Ark 564, although in that case all absorption phases also have flow velocities consistent with zero. This lack of a velocity shift from the rest wavelength agrees with a scenario in which we are observing emission from a fully visible spherically symmetric outflowing shell around the nuclear source, thus no net velocity of O\textsuperscript{vii} will be detected. Another possible explanation is that the O\textsuperscript{vii} line originates in the NLR (described in Sect. 2.2.2), where the emission lines are produced in a gas of comparatively small velocity dispersion and low density (see for e.g. Kaastra et al. (2002), where the forbidden O\textsuperscript{vii} line in NGC 5548 is suggested to come from the NLR). As the forbidden line is the most intense line in the O\textsuperscript{vii} triplet, a photoionised gas with low density is required (see Sect. 3.2.2).

In this chapter tentative evidence for a relativistically broadened emission line of O\textsuperscript{viii} Ly-\textalpha is reported. However, the line is weaker than the strong O\textsuperscript{viii}, N\textsuperscript{vii} and C\textsuperscript{vi} Ly-\textalpha lines reported by Branduardi-Raymont et al. (2001) and Sako et al. (2003) in MCG −6-30-15 and Mrk 766. Evidence for weak broadened emission lines of O\textsuperscript{viii} and N\textsuperscript{vii} Ly-\textalpha is also found in NGC 5548 by Kaastra et al. (2002). The disc inclination angle obtained from my fit to the O\textsuperscript{viii} Ly-\textalpha profile is 33° ± 2. Wu and Han (2001) and Zhang and Wu (2002) have calculated the inclination angles of the BLR (described in Sect. 2.2.1) of several Seyfert 1 galaxies using already published bulge stellar velocity dispersions and black hole masses estimated by reverberation mapping. They calculated an inclination angle of 38.3° ± 7.6 for NGC 3516, which would imply co-planarity of the BLR with the AGN accretion disc.

5.5.4 Intrinsic continuum versus warm absorber variability

The galaxy NGC 3516 has a history of large amplitude continuum variability between observations. Netzer et al. (2002) reported a large drop in flux (factor of ~ 50 at 1 keV) between an ASCA observation in 1994 and a Chandra observation
in 2000. They found that the observed flux and spectral variability at these epochs were consistent with a constant column density of line-of-sight material reacting to changes in the ionising continuum. In the 2006 XMM-Newton data I have found the observed spectral and flux variability to be unrelated to changes in the covering fraction of phase B, unlike what is reported by Turner et al. (2008). Furthermore, the X-ray absorption line depths are sensitive to changes in the covering fraction; however, from close examination of RGS high resolution spectra, there is no evidence to suggest that the covering fraction of phase B changed between observations. I note that the only way the soft X-ray variability from Obs. 2 to Obs. 3 (see Figs. 5.1 and 5.2) may be explained using absorption is by another absorber which is more neutral than the ones detected in the RGS, such that it causes continuum absorption without producing detectable absorption lines in the soft X-ray.

The only parameters that indicate a change during the low flux XMM-Newton Obs. 3 are the ionisation parameter $\xi$ of phase A and the column density $N_H$ of phase B. I find log $\xi \sim 0.9$ and $N_H \sim 3 \times 10^{22}$ cm$^{-2}$ in Obs. 3, whereas in the other three observations they are $\sim 1.0$ and $\sim 2 \times 10^{22}$ cm$^{-2}$, respectively. However, these changes in the warm absorber parameters are very small compared to those in the continuum parameters: power-law slope $\Gamma$ from $\sim 1.8$ to 1.7 in Obs. 3, and normalisation from $\sim 3$ to $2 \times 10^{51}$ photons s$^{-1}$ keV$^{-1}$ at 1 keV; modified blackbody temperature from $\sim 190$ to 210 eV in Obs. 3, and normalisation (emitting area times square root of electron density) from $\sim 1.5$ to $0.5 \times 10^{33}$ cm$^{0.5}$.

The power-law contribution to the continuum heavily outweighs the modified blackbody in all the four observations and is responsible for nearly all of the continuum variability. From the X-ray lightcurve (Fig. 5.1) and spectrum (Fig. 5.2), the variation in Obs. 3 is larger in the soft X-ray (0.2–2.0 keV) energy band than in the hard X-ray (2.0–10.0 keV) band. This type of variability has been seen in other X-ray observations of Seyfert 1 AGN (such as NGC 7469, Blustin et al. 2003), in which the source is softer when brighter. In the next chapter, using a 100-day multi-wavelength campaign on the Seyfert-1 galaxy Mrk 509 and broad-band modelling of the data, I investigate the nature of such X-ray continuum variability in AGN.
Chapter 6

Mrk 509: optical/UV/X-ray variability and the nature of the soft X-ray excess

This chapter is based on Mehdipour et al. (2011), A&A, 534, A39.

In this chapter I present my analysis of XMM-Newton, Swift and HST/COS optical/UV and X-ray observations of the Seyfert-1/QSO Mrk 509, part of an unprecedented multi-wavelength observing campaign, investigating the nuclear environment of this AGN. The XMM-Newton data are from a series of 10 observations of about 60 ks each, spaced from each other by about 4 days, taken in Oct-Nov 2009. During this campaign, Mrk 509 was also observed with Swift for a period of about 100 days, monitoring the behaviour of the source before and after the XMM-Newton observations. With these data I have established the continuum spectrum in the optical/UV and X-ray bands and investigated its variability on the timescale of the campaign with a resolution time of a few days. In order to measure and model the continuum as far as possible into the UV, I also made use of HST/COS observations (part of the Mrk 509 coordinated campaign) and of an archival FUSE observation. I have found that in addition to an X-ray power-law, the spectrum displays soft X-ray excess emission below 2 keV, which interestingly varies in association with the thermal optical/UV emission from the accretion disc. The change in the X-ray power-law component flux (albeit smaller than that of the soft excess), on the other hand, is uncorrelated to the flux variability of the soft X-ray excess and the disc
component on the probed timescale. The results of the simultaneous broad-band spectral and timing analysis suggest that, on a resolution time of a few days, the soft X-ray excess of Mrk 509 is produced by the Comptonisation of the thermal optical/UV photons from the accretion disc by a warm (0.2 keV) optically thick ($\tau \sim 17$) corona surrounding the inner regions of the disc. This makes Mrk 509, with a black hole mass of about $1-3 \times 10^8 M_\odot$, the highest mass known system of its kind to display such behaviour and origin for the soft X-ray excess.

6.1 Introduction

Mrk 509 has a cosmological redshift of 0.034397 (Huchra et al. 1993) corresponding to a luminosity distance of 145 Mpc. The details of the multi-wavelength observing campaign carried out on Mrk 509 in 2009 are presented in Kaastra et al. (2011a). As part of this campaign, Swift monitoring was performed before and after a series of observations by XMM-Newton and the International Gamma-Ray Astrophysics Laboratory (INTEGRAL). One of the aims of this campaign was determining the location of the multi-phase warm absorber outflows (see Sect. 3.6) in Mrk 509; this was done by monitoring the response of the warm absorber (studied using the RGS, Detmers et al. 2011) to intrinsic source variability, i.e. reverberation mapping of the warm absorber (Kaastra, Detmers, Mehdipour et al. 2012). The focus of this chapter is however on the optical/UV and X-ray source variability of Mrk 509 using data mainly from the XMM-Newton OM and EPIC-pn. My goal in this work is to try and explain the intrinsic multi-wavelength variability of Mrk 509 and its relation to the soft X-ray excess in terms of physical changes in the accretion disc and corona.

Past multi-wavelength monitoring campaigns of Seyfert-1 galaxies have shown striking similarities in their optical/UV and X-ray variability, suggesting a strong link between the emissions in these energy ranges, such as that provided by inverse Comptonisation. Walter and Fink (1993) studied the soft X-ray (0.1–2.4 keV) spectra of 58 Seyfert-1 AGN, including Mrk 509, using ROSAT observations. They reported the presence of a soft X-ray excess above the extrapolation of the hard X-ray power-law in 90% of the sources. They also found that the soft X-ray excess is well correlated to the strength of the big-blue-bump observed with the International Ultraviolet Explorer (IUE) in the UV band. They concluded that the big-blue-bump is an ultraviolet-to-soft X-ray feature, which has a similar shape in all Seyfert-1
galaxies of their sample. From an intensive multi-instrument campaign on NGC 4151, Edelson et al. (1996) found that optical/UV and 1–2 keV X-ray fluxes varied together on a timescale of days, with the X-ray flux varying with much larger amplitude than the optical/UV; the phase difference between UV and 1–2 keV X-ray was consistent with zero lag, with an upper limit of \( \lesssim 0.3 \) days. Marshall et al. (1997) measured the spectrum and lightcurve of NGC 5548 over a period of 2 months using the Extreme Ultraviolet Explorer (EUVE) when the galaxy was also monitored with HST. They found the optical/UV and EUV variations to be simultaneous, with the amplitude in the EUV twice that in the UV. Also the shape of the EUVE spectrum was consistent with a gradual decreasing of flux from the UV through to the soft X-ray, with no emission lines detected in the EUV band. Furthermore, from a monitoring study of Mrk 509 using the Rossi X-ray Timing Explorer (RXTE) and ground-based optical observations, Marshall et al. (2008) report a strong correlation between variability of the optical and hard X-ray emission on timescale of a few years, with optical variations leading the hard X-rays by about 15 days.

The structure of this chapter is as follows. In Sect. 6.2 the observations and data analysis are described, Sect. 6.3 focuses on the photometric and spectroscopic corrections applied to the data in order to establish the continuum; the spectral modelling is described in detail in Sects. 6.4 and 6.5 and my findings are discussed in Sect. 6.6. My conclusions and implications of this work are given in Chapter 8.

6.2 Observations and data analysis

For the Mrk 509 multi-wavelength campaign, 5 space telescopes (XMM-Newton, Swift, HST, INTEGRAL and Chandra) and 2 ground-based observatories (WHT and PAIRITEL) were used. Figure 6.1 shows a graphical overview of the timeline of the Mrk 509 campaign.

At the heart of the Mrk 509 campaign, there are a series of 10 XMM-Newton observations of about 60 ks each, spaced from each other by about 4 days, taken in Oct-Nov 2009. Some details of the XMM-Newton’s OM and EPIC-pn observations are shown in Table 6.1. For the OM, the V, B, U, UVW1, UVM2 and UVW2 filters were used during each observation, in order to obtain the best possible characterisation of the SED across the optical/UV bands. For each XMM-Newton observation an optical spectrum using the OM optical grism was also obtained. Observations
6.2. Observations and data analysis

Fig. 6.1: Timeline of the Mrk 509 campaign, spanning over a period of about 100 days. The first observation with Swift started on 4 September 2009, and the last observation with Chandra ended on 13 December 2009.

with the OM UV grism were not allowed for operational reasons. The source was also regularly observed with Swift, before and after the XMM-Newton observations, in order to maintain a continuous monitoring of the source variability in the optical/UV and X-ray bands over the time span of the campaign. The Swift’s UVOT and XRT observations details are shown in Table 6.2. In order to measure and model the continuum as far as possible into the UV (up to the Galactic Lyman limit), I also made use of HST/COS observations of Mrk 509 (part of the coordinated campaign) and of an archival FUSE observation. The HST/COS observations, whose details are given in Table 6.3, were taken about three weeks after the last XMM-Newton observation. The archival FUSE spectrum of Mrk 509 (Obs. ID P1080601) is from a 62.1 ks observation obtained on 5 September 2000.
Table 6.1: The XMM-Newton OM and EPIC-pn observations details of Mrk 509.

<table>
<thead>
<tr>
<th>Obs. ID</th>
<th>yyyy-mm-dd</th>
<th>hh:mm:ss</th>
<th>Start time (UTC)</th>
<th>Total exposure time at each OM filter (ks)</th>
<th>X-ray exposure (ks) a</th>
<th>EPIC-pn</th>
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<td></td>
</tr>
<tr>
<td>0601390301</td>
<td>2009-10-19</td>
<td>15:47:02</td>
<td></td>
<td>V   7.5  B  6.0  U  3.0  UVW1  7.5  UVM2  8.0  UVW2  8.7  Vgrism 5.0</td>
<td>44.4</td>
<td></td>
</tr>
<tr>
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<td>2009-10-23</td>
<td>06:08:12</td>
<td></td>
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<td>42.4</td>
<td></td>
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<tr>
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<td>2009-10-29</td>
<td>07:22:07</td>
<td></td>
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<td>42.4</td>
<td></td>
</tr>
<tr>
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<td>2009-11-02</td>
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<td></td>
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<td></td>
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<td>08:07:05</td>
<td></td>
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aFinal cleaned X-ray exposure times are shown.
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<th>hh:mm:ss</th>
<th>Start time (UTC)</th>
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<td>04:06:41</td>
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<td>0.9</td>
</tr>
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</tr>
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*a Final cleaned X-ray exposure times are shown.
6.2. Observations and data analysis

Table 6.3: The HST/COS observations details of Mrk 509.

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<tr>
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<th>hh:mm:ss</th>
<th>Grating/Tilt</th>
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<td>G160M/1577</td>
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</table>

6.2.1 OM and UVOT broad-band filters data

To calculate the flux density from the count rate at the filter effective wavelengths (Table 4.1 in Sect. 4.3.2), the conversion factors given in XMM-Newton XMM-Newton OM Calibration Status (2011) and Poole et al. (2008) (for the Swift UVOT) were used. Note that these conversion factors have been obtained from observations of standard stars with known spectral shape; therefore the flux of Mrk 509 needs to be corrected for the presence of strong AGN emission lines in the filter bandpasses. I have thus taken into account the contribution to each filter bandpass of all significant emission lines and of the small-blue-bump (see Sect. 6.3.3 for the OM grism modelling) so that the flux at the effective wavelength of the filter corresponds only to the intrinsic continuum emission. For the purpose of spectral fitting with the spex code, the filter count rates and the corresponding response matrices for each of the OM filters were used.

Next, in order to account for the difference in the calibration of the OM and UVOT instruments, I performed the following to normalise the UVOT fluxes against the OM for each filter. As shown in Table 6.1 there are 10 OM observations with exposures in each of the 6 filters. Thus 10 SEDs with 6 optical/UV data points (see Fig. 6.2) were obtained for the source, after implementing all the corrections described in Sect. 6.3. Then a cubic spline interpolation between the data points
Fig. 6.2: The OM SED data points (shown as open circles) for each XMM-Newton observation of Mrk 509. The vertical error bars which represent statistical and systematic uncertainties at 1σ level are mostly within the size of the data symbols. The average spline SED (black curve) obtained from fitting the 10 OM observations is plotted in each panel for reference to show the variability.
for each SED was performed, and thus a flux versus wavelength relation for each OM observation was obtained. During the monitoring campaign there were two occasions when the OM and UVOT observations overlapped (or were very close to overlap). They correspond to OM Obs. 1 and UVOT Obs. 10 (filter M2), and OM Obs. 10 and UVOT Obs. 12 (filter W1). Using the OM SEDs of Obs. 1 and Obs. 10, the expected OM flux at the effective wavelengths of the UVOT M2 and W1 filters was calculated. Then by taking the ratio of the OM and UVOT fluxes, normalisation factors for the M2 and W1 filters of OM and UVOT were obtained. In order to calculate the normalisation factor for the other filters, I made use of UVOT Obs. 2 in which all 6 filters were used. By knowing the average shape of the SED over the duration of the 10 OM observations (see Fig. 6.2) one can scale the SED according to the normalised M2 and W1 fluxes of UVOT Obs. 2. These two SEDs can then be used to give the normalisation factors of the remaining filters assuming the shape of the average OM SED remains the same over the observations. It is found that at the same wavelengths, the OM fluxes are generally larger than the UVOT ones by about 10% due to calibration differences. The time averaged SED also provides a template that can be used to calculate the flux at any particular wavelength for those UVOT observations missing exposures with some of the filters, by knowing only the flux in one of the filters. This assumes that the shape of the average OM SED is a good representation of the source and did not change during the Swift observations, which are before and after the 37-day time span of the OM observations. So finally, the lightcurves in Fig. 6.3 show how the OM and UVOT continuum fluxes measured at the same wavelengths (effective wavelength of the OM filters, shown above each panel in Fig. 6.3) varied over the combined 100 days duration of the XMM-Newton and Swift observations.

### 6.2.2 HST/COS and archival FUSE data

Since both COS and FUSE share a common wavelength band from about 1165 to 1185 Å, the archival FUSE spectrum was easily scaled to the flux level at the time of the COS observations, assuming the continuum shape in the FUSE band did not vary. The mean COS and FUSE spectra of Mrk 509, corrected for Galactic extinction, are shown in Fig. 6.4. For the purpose of broad-band modelling of Mrk 509, I used measurements of the UV continuum from narrow spectral bands, which are free of emission and absorption lines (see Table 6.4). The COS observations were
6.2. Observations and data analysis

Fig. 6.3: Intrinsic optical/UV continuum lightcurves of Mrk 509 over a period of 100 days at the end of 2009 at the wavelengths indicated above each panel. Blue squares: OM; red circles: measured UVOT; green triangles: UVOT observations for which fluxes have been calculated using a time-averaged SED as described in Sect. 6.2.1. The error bars of all lightcurves represent statistical and systematic calibration uncertainties at 1σ level.

made close in time to the UVOT Obs. 18, and since UVOT Obs. 18 is close in flux level to that of OM Obs. 2, the COS and the FUSE data were included when modelling the XMM-Newton Obs. 2 data. For all other XMM-Newton observations, the COS and FUSE data were scaled based on the flux level observed in the OM optical/UV filters.
Fig. 6.4: HST/COS (shown in red) and FUSE (shown in blue) UV spectra of Mrk 509. The spectra are corrected of Galactic extinction and are displayed in the observed frame. The FUSE observations were taken on 5 September 2000 and the COS observations are from 10-11 December 2009. The FUSE spectrum has been normalised to the flux level of COS. Some of the prominent broad emission features are labelled. For the study of intrinsic UV absorption in Mrk 509 see Kriss et al. (2011). Measurements of the UV continuum (Table 6.4) taken from narrow spectral bands, which are free of emission and absorption lines, have been used in this work for my broad-band modelling of Mrk 509. COS and FUSE data courtesy of Gerard A. Kriss.
6.3 Intrinsic continuum emission

In order to establish the intrinsic continuum emission of Mrk 509, photometric and spectroscopic corrections were applied to the data to take into account the processes which take place in our line of sight towards the central engine. Sects. 6.3.1, 6.3.2 and 6.3.3 are applicable to the optical/UV (OM and UVOT), and Sects. 6.3.4 and 6.3.5 to the X-ray (EPIC-pn and XRT). In the latter case the presence of Galactic and AGN warm absorption is taken into account during the fitting process.

6.3.1 Galactic interstellar dereddening

To correct the OM and UVOT optical/UV fluxes for interstellar reddening in our Galaxy, the reddening curve of Cardelli et al. (1989) was used, including the update for near-UV given by O'Donnell (1994). The colour excess \( E(B - V) = 0.057 \) mag is based on calculations of Schlegel et al. (1998) as shown in the NASA/IPAC Extragalactic Database (NED). The scalar specifying the ratio of total to selective extinction \( R_V \equiv A_V/E(B - V) \) was fixed at 3.1.

6.3.2 Host galaxy stellar emission

To correct for the host galaxy starlight contribution in the OM and UVOT fields I have used the results of Bentz et al. (2009) and Kinney et al. (1996). Bentz et al. (2009) have determined the host galaxy observed flux at the rest-frame wavelength

Table 6.4: The FUSE and HST/COS continuum flux values of Mrk 509 corrected for Galactic extinction. The FUSE observations were taken on 5 September 2000 and the COS observations are from 10-11 December 2009. The FUSE values have been normalised to the COS level.

<table>
<thead>
<tr>
<th>Instrument</th>
<th>Band (Å)</th>
<th>( F_\lambda ) (erg cm(^{-2}) s(^{-1}) Å(^{-1}))</th>
<th>Flux error</th>
</tr>
</thead>
<tbody>
<tr>
<td>FUSE</td>
<td>941 – 944</td>
<td>( 2.15 \times 10^{-13} )</td>
<td>10%</td>
</tr>
<tr>
<td>FUSE</td>
<td>959 – 961</td>
<td>( 1.93 \times 10^{-13} )</td>
<td>10%</td>
</tr>
<tr>
<td>FUSE</td>
<td>983 – 985</td>
<td>( 1.87 \times 10^{-13} )</td>
<td>10%</td>
</tr>
<tr>
<td>FUSE</td>
<td>992 – 994</td>
<td>( 1.72 \times 10^{-13} )</td>
<td>10%</td>
</tr>
<tr>
<td>FUSE/COS</td>
<td>1165 – 1185</td>
<td>( 1.68 \times 10^{-13} )</td>
<td>5%</td>
</tr>
<tr>
<td>COS</td>
<td>1405 – 1425</td>
<td>( 1.47 \times 10^{-13} )</td>
<td>5%</td>
</tr>
<tr>
<td>COS</td>
<td>1740 – 1760</td>
<td>( 1.07 \times 10^{-13} )</td>
<td>5%</td>
</tr>
</tbody>
</table>
6.3. Intrinsic continuum emission

Fig. 6.5: The calculated bulge stellar spectrum of Mrk 509 host galaxy shown in the range covered by the OM optical grism. The spectrum is normalised with the HST measurement at rest wavelength of 5100 Å given in Bentz et al. (2009) and is obtained by using the bulge model template of Kinney et al. (1996) to calculate the flux at other wavelengths. The two data points (green crosses) superimposed on the spectrum are the nuclear stellar flux for the standard B and V filters measured by Kotilainen and Ward (1994); the horizontal bars represent the filter bandpasses.

of 5100 Å ($F_{\text{gal}, 5100 \, \text{Å}}$) for a sample of AGN using HST images. For Mrk 509, $F_{\text{gal}, 5100 \, \text{Å}} = (2.52 \pm 0.23) \times 10^{-15}$ erg s$^{-1}$ cm$^{-2}$ Å$^{-1}$ for an aperture of 5.0$''$ x 7.6$''$. In order to calculate the host galaxy spectrum in the optical band, I used a model spectrum and scaled it based on the $F_{\text{gal}, 5100 \, \text{Å}}$ value. Since the OM and UVOT apertures are taking in only the galaxy’s innermost few kpc, the galaxy bulge template of Kinney et al. (1996) was used. Figure 6.5 shows the host bulge model spectrum in the optical band, which becomes gradually negligible going towards the UV.

Kotilainen and Ward (1994) have also measured the nuclear stellar flux contribution using different broad-band filters in a 6$''$ diameter circular aperture for a sample of galaxies. They have done this by subtracting the AGN contribution using profile fitting. The nuclear stellar flux of Mrk 509 for the standard B and V filters are shown in Fig. 6.5 and appear consistent with the host bulge model spectrum.
6.3. Intrinsic continuum emission

Fig. 6.6: The observed OM optical grism spectrum of Mrk 509 (already corrected for Galactic extinction and the AGN host galaxy stellar emission) obtained by averaging the OM optical grism spectra from the 10 XMM-Newton observations. The data are shown in black and the model described in Sect. 6.3.3 in red. The prominent broad and narrow emission features are labelled. The low-level sinusoidal pattern below 3900 Å is a residual effect of the Modulo-8 fixed pattern noise.

6.3.3 Correction for emission from the BLR and NLR

For each of the 10 XMM-Newton observations, there is a 5 ks OM optical grism exposure available, with which one can model emission from the BLR and NLR (described in Sect. 2.2). Figure 6.6 shows the mean optical grism spectrum of the observations and a fitted model. The accretion disc blackbody model spectrum (used in Sect. 6.4.2 and shown for example in Fig. 6.11) has a power-law shape in the optical band. Thus, to model the underlying optical continuum (3000–7000 Å) in the OM grism spectra I used a simple power-law rather than a disc blackbody model, which requires a wider energy band to be fitted properly. The main purpose in fitting the OM grism is modelling the emission features and therefore a simple continuum model is preferred (see Sect. 6.4.2 for the modelling of the optical/UV continuum with the OM image data). As shown in Fig. 6.6 there is excess emission below about 4000 Å which is likely to be the long-wavelength end of the “small-blue-bump” feature (see Sect. 2.2.1). Note that the low-level sinusoidal pattern below 3900 Å in Fig. 6.6 is an instrumental effect (residual of the Modulo-8 fixed pattern noise; Mason et al. 2001), although the overall average flux level is correct. The
6.3. Intrinsic continuum emission

Table 6.5: Best-fit parameters of the broad and narrow emission features in the mean OM optical grism spectrum of Mrk 509. The \( \chi^2_\nu = 1.04 \) (302 d.o.f.).

<table>
<thead>
<tr>
<th>Emission</th>
<th>Energy flux (^a) (10(^{-13}) erg s(^{-1}) cm(^{-2}))</th>
<th>FWHM (^b) (km s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(\alpha) (\lambda 6563)</td>
<td>44 ± 2</td>
<td>4300 ± 200</td>
</tr>
<tr>
<td>H(\beta) (\lambda 4861)</td>
<td>17.0 ± 0.5</td>
<td>4400 ± 200</td>
</tr>
<tr>
<td>H(\gamma) (\lambda 4340)</td>
<td>9.0 ± 0.3</td>
<td>4400 ± 200</td>
</tr>
<tr>
<td>H(\delta) (\lambda 4101)</td>
<td>4.2 ± 0.3</td>
<td>3700 ± 300</td>
</tr>
<tr>
<td>[O(\text{III})] (\lambda 4959)</td>
<td>2.2 ± 0.3</td>
<td>1100 ± 200</td>
</tr>
<tr>
<td>[O(\text{III})] (\lambda 5007)</td>
<td>7.8 ± 0.3</td>
<td>1500 ± 200</td>
</tr>
<tr>
<td>small-blue-bump</td>
<td>44 ± 5 (^c)</td>
<td>-</td>
</tr>
</tbody>
</table>

\(^a\) 10\(^{-13}\) erg s\(^{-1}\) cm\(^{-2}\).
\(^b\) km s\(^{-1}\).
\(^c\) Calculated between 2900 and 3700 Å rest-wavelength.

spectral shape of the small-blue-bump is strongly blended and thus this complex feature was modelled with a cubic spline with linear spacing between 3000 and 4000 Å (in the observed frame) and 10 grid points. The broad and narrow emission lines were modelled using Gaussian line profiles. The best-fit parameters of the emission features are shown in Table 6.5.

Furthermore, having obtained a best-fit model for the mean spectrum, I applied it to the individual observations and subsequently fitted them. This makes it possible to look for any changes in the emission lines during the XMM-Newton campaign (\(\sim 37\) days) and see how they behave with respect to the continuum variability. I did not detect any statistically significant variation in the lines like observed for the continuum (see Fig. 6.3). This is consistent with the results of the monitoring program of Mrk 509 by Carone et al. (1996) who found the H\(\beta\) \(\lambda 4861\) and He\(\text{II}\) \(\lambda 4686\) emission lines to respond to continuum variations with time lags of about 80 and 60 days respectively, considerably longer than the emission line lags measured for other Seyfert galaxies and also longer than the duration of the XMM-Newton campaign on Mrk 509. Finally, I proceeded to correct the OM and UVOT filter data (described in Sect. 6.2.1) for the emission feature contributions in the different filter bands.
6.3.4 Galactic interstellar X-ray absorption correction

In my modelling of the X-ray spectra of Mrk 509 the effects of the Galactic neutral absorption were included by applying the hot model (introduced in Sect. 3.4) in spex. Assuming Lodders (2003) abundances, the Galactic HI column density in our line of sight was fixed to $N_H = 4.44 \times 10^{20} \text{ cm}^{-2}$ (Murphy et al. 1996) and the gas temperature to 0.5 eV to mimic a neutral gas in collisional ionisation equilibrium.

6.3.5 Warm absorber correction

In order to perform a multi-wavelength intrinsic variability study one also needs to determine the X-ray continuum before absorption by the AGN warm absorber. To this end, the spex xabs (see Sect. 3.4) photoionised absorption model was used, with the parameters of Detmers et al. (2011) derived for the stacked 600 ks RGS spectrum gathered during the XMM-Newton campaign. Note that the correction for absorption by the warm absorber is too small to account for the observed X-ray variability. The warm absorption correction is less than 6% of the X-ray photon flux in all the observations, whereas from Obs. 1 to Obs. 5 the photon flux increases by about 45%.

6.4 Independent modelling of the X-ray and optical/UV continua

In this section my modelling of the optical/UV (OM) and X-ray spectra (EPIC-pn) of Mrk 509, fitted independently of each other, is described. In the next section (Sect. 6.5), simultaneous broad-band fits are performed with my final model. Note that all the photometric and spectroscopic corrections described in the previous section, and the cosmological redshift have been taken into account here. All the fitted parameter errors quoted in this chapter correspond to a $\Delta \chi^2$ of 1 (68.3% confidence level for one interesting parameter). Parameters of the models given in the tables correspond to the source reference frame, whereas all the figures in this chapter are displayed in the observed frame.

6.4.1 The X-ray continuum and Fe Kα line

The EPIC-pn spectra of Obs. 1 and Obs. 5 are shown together in Fig. 6.7 to display the extremes of the X-ray variability observed in Mrk 509 during the XMM-Newton campaign. The spectral modelling was begun by fitting the EPIC-pn 0.3–10 keV
6.4. Independent modelling of the X-ray and optical/UV continua

Fig. 6.7: Mrk 509 EPIC-pn spectra of Obs. 1 (magenta) and Obs. 5 (blue) binned to a minimum of 100 counts per bin. The spectrum of Obs. 5 has a higher flux than that of Obs. 1 at low energies.

X-ray continuum and the Fe Kα line at ∼ 6.4 keV of Obs. 1 with a simple power-law (POW in SPEX) and a Gaussian line profile (GAUS in SPEX) including the absorption models described in Sects. 6.3.4 and 6.3.5. I found that a single power-law cannot fit the continuum well between 0.3–10 keV because of the presence of a soft excess below about 2 keV. For a single power-law fit over 0.3–10 keV a Γ of 2.27 and a χ²ν of 7.9 (1788 d.o.f.) are obtained, whereas for a fit between 2.5–10 keV, Γ = 1.79 and χ²ν = 1.01 (1353 d.o.f.). Figure 6.8 shows the 2.5–10.0 keV EPIC-pn fit for Obs. 1, extrapolated to lower energies, clearly displaying the presence of a steeper continuum below about 2 keV.

The 0.3–10 keV continuum of Obs. 1 was then fitted by adding a second power-law component to model the soft excess, which resulted in a best-fit with χ²ν of 1.09 (1786 d.o.f.). The photon indices of the two power-laws are significantly different: Γ = 2.75 for the soft X-ray component and Γ = 1.46 for the hard one. Figure 6.9 shows the two power-law best-fit to the data of Obs. 1. This model was then applied to the spectra of all 10 EPIC-pn observations. Table 6.6 shows the best-fit parameters for the two power-law model for each observation.

The subject of this work is the broad-band modelling of the Mrk 509 continuum, so I have represented the Fe Kα line with a simple Gaussian profile
6.4. Independent modelling of the X-ray and optical/UV continua

**Fig. 6.8:** Mrk 509 Obs. 1 EPIC-pn single power-law fit (including a Gaussian Fe Kα line, Galactic and warm absorption) over the 2.5–10 keV range. The fit is extrapolated to lower energies, displaying the presence of a soft excess below about 2 keV. The data are shown in black and model in red. Residuals of the fit, (Observed−Model)/Model, are displayed in the bottom panel.

**Fig. 6.9:** Mrk 509 Obs. 1 EPIC-pn two power-law fit (including a Gaussian Fe Kα line, Galactic and warm absorption) over the 0.3–10 keV range. The data are shown in black and model in red. Residuals of the fit, (Observed−Model)/Model, are displayed in the bottom panel.
which gives a good fit. For an in-depth analysis and modelling of the Fe Kα band in Mrk 509, the reader is referred to Ponti et al. (in press), in which data from the long Mrk 509 campaign are used to study the profile and variability of the Fe Kα line in great detail. The parameters of the Fe Kα line, fitted using a single Gaussian profile, for the summed EPIC-pn spectrum are: line energy $E = 6.43 \pm 0.01$ keV, width $\sigma = 0.14 \pm 0.02$ keV, EW $= 70 \pm 5$ eV and normalisation of $(3.8 \pm 0.3) \times 10^{-5}$ photons cm$^{-2}$ s$^{-1}$. From previous XMM-Newton and Suzaku observations of Mrk 509 reported by Ponti et al. (2009), the shape of the neutral Fe Kα line does not show signs of relativistic distortions. Using EPIC-pn data from the 2009 campaign, from reverberation measurement of the Fe Kα line (with no measurable lag present) and lack of a redshifted wing in the line, Ponti et al. (in press) infer a location for the bulk of the emission at a distance of $\sim 40–1000 \ R_g$ from the SMBH (with the gravitational radius $R_g = GM/c^2$, where $G$ is the gravitational constant, $M$ the mass of the black hole and $c$ the speed of light).

Next, the Swift XRT spectra of Mrk 509 were examined to get a measure of
the X-ray flux before and after the XMM-Newton campaign. However, one needs to note that the XRT exposures are very short at around 1 ks (see Table 6.1), and also the effective area of the XRT is very much lower than that of EPIC-pn; thus the XRT spectra are of low statistical quality, and do not allow performing any accurate spectral modelling. Therefore, instead of reporting parameters of the XRT fits, in Fig. 6.10 I show how the soft X-ray (0.3 keV) and hard X-ray (4 keV) continuum fluxes varied for both XRT and EPIC-pn over the 100 days duration of the Mrk 509 campaign.

6.4.2 The optical/UV continuum

Apart from line emission from the BLR and NLR (which has been taken into account in my continuum modelling of Mrk 509 - see Sect. 6.3.3), the dominant feature of the optical/UV spectra of AGN is the big-blue-bump, which is attributed to thermal emission from the accretion disc (see Sect. 2.1). To fit the big-blue-bump of Mrk 509, I applied the dbb disc blackbody model in spex, which is based on a geometrically thin, optically thick Shakura-Sunyaev accretion disc (Shakura and Sunyaev 1973) to the OM, HST/COS and FUSE data. The fitted parameters of the model are the normalisation $A$ and the maximum temperature of the disc $T_{\text{max}}$. The radius of the outer edge of the disc was fixed to $10^3 R_{\text{in}}$, where $R_{\text{in}}$ is the radius at the inner edge of the disc.

Table 6.7 shows the best-fit parameters of the disc blackbody model for each XMM-Newton observation. $T_{\text{max}}$ increases from its minimum in Obs. 1 to its maximum in Obs. 5 and then gradually decreases back to the level of Obs. 1 towards the end of the XMM-Newton campaign. The normalisation area of the disc blackbody remains unchanged within errors, which implies that $R_{\text{in}}$ and inclination $i$ parameters have not significantly varied. Thus one can infer that the variability in the disc temperature comes from a change in the accretion rate. Figure 6.11 shows the OM SED data points and their corresponding disc blackbody best-fit models, and also the EPIC-pn two power-law best-fit models of Sect. 6.4.1 for all 10 XMM-Newton observations.

So far the optical/UV and X-ray data have been modelled independently of each other; in Sect. 6.5 I make simultaneous fits to both data sets in order to establish a model that accounts for the broad-band spectrum of Mrk 509 and for its observed variability.
6.4. Independent modelling of the X-ray and optical/UV continua

**Fig. 6.10:** X-ray continuum flux lightcurves of Mrk 509 over 100 days in 2009 at 0.3 keV (top panel) and 4.0 keV (bottom panel). The red circles (with large error bars) represent the XRT points and the blue squares represent the EPIC-pn points. The bandwidths used to calculate the 0.3 keV fluxes are 0.02 keV for EPIC-pn and 0.3 keV for XRT, and the bandwidths used to calculate the 4.0 keV fluxes are 0.1 keV for EPIC-pn and 2.0 keV for XRT.
Fig. 6.11: The Mrk 509 best-fit model derived in Sect. 6.4 independently for the optical/UV and X-ray bands for each XMM-Newton observation. The absorption-corrected EPIC-pn data are shown in green and the black lines are the two power-law model fits to the EPIC-pn including a Gaussian for modelling the Fe Kα line. The red circles represent the OM data and the blue lines are the disc blackbody models. In panel 2, the purple squares are the HST/COS data and the brown diamonds are the scaled FUSE data. The average model obtained from the 10 XMM-Newton observations is shown in each panel (in grey) for reference to show the variability.
Table 6.7: Best-fit parameters of the optical/UV continuum of Mrk 509, obtained from a
disc blackbody model fit to the OM data of each observation as described in Sect. 6.4.2.

<table>
<thead>
<tr>
<th>Obs.</th>
<th>$T_{\text{max}}$ $^a$</th>
<th>Norm $^b$</th>
<th>$\chi^2 / \text{d.o.f.}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.82 ± 0.06</td>
<td>6.9 ± 0.6</td>
<td>0.6/11</td>
</tr>
<tr>
<td>2</td>
<td>3.89 ± 0.06</td>
<td>6.7 ± 0.6</td>
<td>0.6/11</td>
</tr>
<tr>
<td>3</td>
<td>3.94 ± 0.07</td>
<td>6.6 ± 0.6</td>
<td>0.6/11</td>
</tr>
<tr>
<td>4</td>
<td>4.08 ± 0.08</td>
<td>6.2 ± 0.6</td>
<td>0.8/11</td>
</tr>
<tr>
<td>5</td>
<td>4.15 ± 0.08</td>
<td>6.0 ± 0.6</td>
<td>0.8/11</td>
</tr>
<tr>
<td>6</td>
<td>4.00 ± 0.07</td>
<td>6.5 ± 0.6</td>
<td>0.6/11</td>
</tr>
<tr>
<td>7</td>
<td>3.95 ± 0.07</td>
<td>6.6 ± 0.6</td>
<td>0.6/11</td>
</tr>
<tr>
<td>8</td>
<td>3.86 ± 0.06</td>
<td>6.9 ± 0.6</td>
<td>0.6/11</td>
</tr>
<tr>
<td>9</td>
<td>3.94 ± 0.07</td>
<td>6.5 ± 0.6</td>
<td>0.7/11</td>
</tr>
<tr>
<td>10</td>
<td>3.86 ± 0.06</td>
<td>6.9 ± 0.6</td>
<td>0.6/11</td>
</tr>
</tbody>
</table>

$^a$ Maximum temperature in the disc in eV.
$^b$ Normalisation area ($A = R_{\text{in}}^2 \cos i$) in $10^{28} \text{cm}^2$.

6.4.3 Correlation between optical/UV and X-ray count rates

Figure 6.10 (EPIC-pn blue square data points in the top panel) indicates that the
soft X-ray continuum flux of Mrk 509 varied over the 10 XMM-Newton observations
in a very similar fashion to the optical/UV continuum (OM blue square data points
in Fig. 6.3). In order to explore the link between the optical/UV and X-ray emis-
sion in a model-independent way, I looked at the correlation between their count
rates. Fig. 6.12 shows the UV (2120 Å) count rate plotted against the 0.3 keV soft
X-ray count rate (top panel) and the 0.3 keV soft X-ray excess flux (bottom panel)
for the 10 XMM-Newton observations. Furthermore, the correlation coefficients be-
tween the optical/UV and X-ray count rates are given in Fig. 6.13, demonstrating a
significant correlation at soft X-ray energies. In fact this correlation is as strong as
the one between the UV and optical count rates: the Pearson correlation coefficient
between the count rates in the UV and optical filters is about 0.85, which is sta-
tistically significant with probability of no correlation $p = 0.002$ from the Student’s
t-test. As shown in Fig. 6.13 the correlation between the optical/UV and X-ray
count rates becomes weaker as the X-ray energy gets larger. So the correlation is
6.4. Independent modelling of the X-ray and optical/UV continua

Fig. 6.12: Top panel: The UV (2120 Å) count rate from the OM UVW2 filter plotted versus the EPIC-pn soft X-ray (0.3 keV) count rate for the 10 XMM-Newton observations of Mrk 509. The bandwidth used for the 0.3 keV bin is 0.02 keV. Bottom panel: The UV (2120 Å) count rate from the OM UVW2 filter plotted versus the EPIC-pn soft X-ray excess flux at 0.3 keV (power-law subtracted soft X-ray flux using the broadband modelling described in Sect. 6.5) for the 10 XMM-Newton observations of Mrk 509. The bandwidth used for the 0.3 keV bin is 0.02 keV.

Indeed strongest at those X-ray energies where the soft excess emission is strongest (below \( \sim 1 \text{ keV} \)), implying a tight link between the optical/UV and the soft X-ray excess emissions. I investigate this further in the next section by applying a broad-band model to all the data.
6.5 Broad-band modelling of the continuum using Comptonisation

The results of the previous section suggest that the continua in the optical/UV and soft X-ray bands may be physically related, i.e. they may be the results of an underlying process linking the two. Comptonisation up-scattering the optical/UV photons to X-ray energies could be such a process (see Sect. 2.3.1). Thus the COMT component in spex was applied to fit the optical/UV and X-ray data simultaneously. The seed photons temperature $T_{\text{seed}}$ were coupled to the disc temperature $T_{\text{max}}$ which was left as a free parameter in the broad-band fitting. The up-scattering Comptonising plasma was chosen to have a disc geometry; its parameters are the temperature $T_e$ and the optical depth $\tau$. The COMT component assumes spherical symmetry for the
6.6 Discussion

6.6.1 Broad-band continuum variability

Optical/UV continuum lightcurves of Mrk 509 (Fig. 6.3) display very similar variability in the 6 filters during the 100 days total duration of the Swift and XMM-Newton campaigns. Specifically, during the 10 XMM-Newton observations, the optical/UV continuum smoothly increased from its minimum in Obs. 1 to its maximum in Obs. 5 (18 days after Obs. 1) and then gradually decreased returning to almost the level of Obs. 1 towards the end of the XMM-Newton campaign. In Sect. 6.4.3 it was shown that there is a strong model-independent correlation between

flux calculation. As for my modelling in Sect. 6.4, all the absorption and emission corrections discussed in Sect. 6.3 and the cosmological redshift, were implemented in the modelling here. In addition to the Comptonisation component which models the optical/UV continuum and the soft X-ray excess, a power-law component and a Gaussian line were also included to represent the hard X-ray continuum and the Fe Kα line; the power-law was smoothly broken at low energies to avoid overshooting the optical/UV flux of the disc blackbody and becoming unphysical. In one of a series of papers on the Mrk 509 campaign (Petrucci et al. in press), higher energy INTEGRAL data are also included in the broad-band spectral fitting, and the hard X-ray continuum is modelled by Comptonisation of the disc photons in a hot corona, instead of using a power-law model as done here. In my work, however, I focus on the direct relation between the disc blackbody emission and the soft X-ray excess and an adequate but simpler representation of the higher energy part of the spectrum is preferred. Table 6.8 shows the best-fit parameters of my broad-band model for each XMM-Newton observation.

Figure 6.14 shows the best-fit broad-band Comptonisation model for XMM-Newton Obs. 2, displaying individual components contributing to the total model spectrum. Figure 6.15 shows luminosity of the X-ray power-law (top panel) and luminosity of the Comptonisation component (bottom panel) plotted versus the disc blackbody bolometric luminosity for the 10 XMM-Newton observations. Interestingly, there is a strong linear correlation between the soft excess modelled by warm Comptonisation and the disc emission, whereas there is no such obvious correlation between the power-law and the disc emission.
6.6. Discussion

Fig. 6.14: Best-fit broad-band model for \textit{XMM-Newton} Obs. 2 of Mrk 509 as described in Sect. 6.5. The red circles represent the OM data, the purple squares the HST/COS data, the brown diamonds are the scaled FUSE data and in green are the absorption-corrected EPIC-pn data. The grey line is the disc blackbody component, the dashed magenta is the warm Comptonisation component and the olive colour line represents the broken power-law and includes a Gaussian for modelling the Fe Kα line. The black line is the total model spectrum.

The optical/UV and soft X-ray flux, whereas there is lack of correlation between the optical/UV and hard X-ray data (see Figs. 6.12 and 6.13). Similarly, using my best-fit broad-band model, Fig. 6.15 indicates a strong linear correlation between the luminosity of the disc blackbody and that of the Comptonised soft X-ray excess: 
\[ L_{\text{soft excess}} = 0.448 L_{\text{disc}} - 1.007, \]
where the luminosities are in units of \(10^{44}\) erg s\(^{-1}\). However, there is no obvious correlation between the luminosity of the disc and that of the X-ray power-law component. The computed Pearson correlation coefficient between the luminosity of the disc and the Comptonised soft excess component is +0.97 (which is statistically significant with probability of no correlation \(p = 10^{-5}\)), and between the disc and the X-ray power-law is +0.09 (which is not significant with \(p = 0.81\)). Also using the luminosities calculated from the broad-band modelling in Sect. 6.5, the correlation coefficient between the X-ray luminosity of the Comptonised soft excess and the power-law is +0.17 (\(p = 0.63\)), which suggests
6.6. Discussion

Fig. 6.15: Top panel: the best-fit X-ray power-law luminosity calculated between 0.2–10 keV, plotted versus the disc blackbody bolometric luminosity for the 10 XMM-Newton observations. Bottom panel: 0.2–10 keV luminosity of the soft excess modelled by warm Comptonisation, plotted versus the disc blackbody bolometric luminosity for the 10 XMM-Newton observations. The luminosities are obtained from the broad-band modelling described in Sect. 6.5. The blue line in the bottom panel is a fit to the luminosities with linear model: $L_{\text{soft excess}} = 0.448 L_{\text{disc}} - 1.007$, where the luminosities are in units of $10^{44}$ erg s$^{-1}$. 
### Table 6.8: Best-fit parameters of the broad-band warm Comptonisation modelling described in Sect. 6.5 for each XMM-Newton observation of Mrk 509.

<table>
<thead>
<tr>
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<tbody>
<tr>
<td></td>
<td>( T_{\text{max}} ) (^a)</td>
<td>Norm (^b)</td>
<td>( T_{\text{seed}} ) (^c)</td>
<td>( T_{\text{e}} ) (^d)</td>
</tr>
<tr>
<td>1</td>
<td>1.96 ± 0.07</td>
<td>3.9 ± 0.8</td>
<td>1.96 (c)</td>
<td>0.21 ± 0.01</td>
</tr>
<tr>
<td>2</td>
<td>2.02 ± 0.07</td>
<td>3.7 ± 0.8</td>
<td>2.02 (c)</td>
<td>0.22 ± 0.01</td>
</tr>
<tr>
<td>3</td>
<td>2.16 ± 0.07</td>
<td>3.1 ± 0.7</td>
<td>2.16 (c)</td>
<td>0.19 ± 0.01</td>
</tr>
<tr>
<td>4</td>
<td>2.26 ± 0.09</td>
<td>2.8 ± 0.7</td>
<td>2.26 (c)</td>
<td>0.19 ± 0.01</td>
</tr>
<tr>
<td>5</td>
<td>2.36 ± 0.09</td>
<td>2.5 ± 0.8</td>
<td>2.36 (c)</td>
<td>0.19 ± 0.01</td>
</tr>
<tr>
<td>6</td>
<td>2.13 ± 0.08</td>
<td>3.4 ± 0.8</td>
<td>2.13 (c)</td>
<td>0.19 ± 0.01</td>
</tr>
<tr>
<td>7</td>
<td>2.07 ± 0.07</td>
<td>3.6 ± 0.7</td>
<td>2.07 (c)</td>
<td>0.19 ± 0.01</td>
</tr>
<tr>
<td>8</td>
<td>2.01 ± 0.07</td>
<td>3.9 ± 0.8</td>
<td>2.01 (c)</td>
<td>0.21 ± 0.01</td>
</tr>
<tr>
<td>9</td>
<td>2.18 ± 0.08</td>
<td>2.9 ± 0.7</td>
<td>2.18 (c)</td>
<td>0.21 ± 0.01</td>
</tr>
<tr>
<td>10</td>
<td>1.99 ± 0.07</td>
<td>3.9 ± 0.8</td>
<td>1.99 (c)</td>
<td>0.20 ± 0.01</td>
</tr>
</tbody>
</table>

\(^a\) Maximum temperature in the disc in eV.
\(^b\) Normalisation area \((A = R_{\text{in}}^2 \cos i)\) in \(10^{29}\) cm\(^2\).
\(^c\) Temperature of the seed photons in eV (coupled to \( T_{\text{max}} \)).
\(^d\) Warm corona temperature in keV.
\(^e\) Optical depth.
\(^f\) \(10^{52}\) photons s\(^{-1}\) keV\(^{-1}\) at 1 keV.
\(^g\) Photon index.
that the fluxes from the two components are not linked over the probed timescales. However, there is a significant correlation with coefficient $+0.88$ ($p = 10^{-3}$) between the power-law photon index (given in Table 6.8) and the disc blackbody luminosity. This behaviour is similar to NGC 7469 (Nandra et al. 2000) in which the UV flux and the hard X-ray photon index were correlated but the UV and hard X-ray fluxes were uncorrelated (like in Mrk 509). Furthermore, on much longer timescales (few years), Marshall et al. (2008) have found a correlation between optical and RXTE hard X-ray data. In general, correlations between different energy bands depend on the timescales and resolutions of the monitoring observations.

6.6.2 The origin of the soft X-ray excess

Here I discuss different interpretations for the origin of the soft X-ray excess, and discuss why Comptonisation is the most likely explanation for its presence in Mrk 509.

One of the early explanations for the soft X-ray excess emission in AGN was its identification with the high energy tail of thermal emission from the accretion disc (e.g. Arnaud et al. 1985, Pounds et al. 1986). As shown in Fig 6.11, it is evident that in the case of Mrk 509 the disc blackbody emission from a geometrically thin, optically thick Shakura-Sunyaev disc, cannot extend to the soft X-ray band. Often it is not possible to measure the peak of the disc emission for AGN as it falls in the EUV gap. The peak temperature of the disc scales with the mass of the black hole as $M^{-1/4}$, and so more massive black holes tend to have lower disc temperatures. The disc blackbody emission of Mrk 509, which has a relatively high black hole mass of $1–3 \times 10^8 M_\odot$ (see Sect. 6.6.3), has a low temperature, which causes the peak of the big-blue-bump to be in the detection range of the HST/COS.

Another interpretation of the soft X-ray excess in AGN is given by Gierliński and Done (2004), who suggest it could be an artefact of absorption by a relativistically smeared, partially ionised disc wind. They analysed publicly available XMM-Newton EPIC spectra of 26 radio-quiet Palomar-Green (PG) quasars and initially modelled the soft X-ray excess with a Comptonisation component. They found a similar Comptonising region temperature (0.1 to 0.2 keV) for the whole sample, which they claim to be puzzling since the objects in their sample have a large range in mass and luminosity, and hence disc temperature. For this reason they suggest the soft X-ray excess may not be real emission, and propose
an alternative solution based on absorption. This relativistically smeared ionised absorption was modelled with xstar \cite{Bautista_2001}, convolved with a Gaussian velocity dispersion of $\sim 0.2c$. \cite{Gierlinski_2004} suggest that the smearing is such that it eliminates the possibility of detecting any absorption lines in the RGS spectrum. The absorption creates a wide dip in the EPIC spectrum around 1 keV which results in an apparent soft excess at lower energies. However, it is worth noting that by fitting the soft X-ray excess using Comptonisation, there is inevitably large uncertainty in constraining the parameters of the plasma when using only EPIC data as there is degeneracy in the fitting process. In fact, excluding the optical/UV data I can get a good fit to the EPIC data of Mrk 509 with a range of values for the plasma parameters from $T_e = 0.2\text{keV}$ and $\tau = 18$ to $T_e = 1.0\text{keV}$ and $\tau = 6$. Therefore, broad-band modelling of simultaneous optical to X-ray data including the peak of the big-blue-bump emission (as performed in this work) is essential to constrain the parameters of the Comptonisation. In most AGN, however, the peak falls in the EUV band where there are no data available, which causes more uncertainty when modelling. Using a small energy window for modelling can lead to a small scatter in the parameters of the plasma; only broad-band observations can show the real scatter. Moreover, \cite{Gierlinski_2004} have constrained their model for all the AGN in their sample by fixing the disc blackbody temperature at 10 eV, the temperature of the hot component at 100 keV and the photon index of the component used to fit the soft X-ray band at 2. These constraints would have an impact on the best-fit results. Furthermore, variability of the soft X-ray excess is crucial in understanding its origin; from my broad-band variability study of Mrk 509, using both EPIC and OM data (together with the HST/COS and FUSE UV measurements), the soft X-ray excess is found to be ‘real’ emission, which varies in a similar fashion to the disc emission.

The soft X-ray excess has also been associated with the relativistically blurred photoionised disc reflection model of \cite{Ross_2005}. According to this model, the X-ray power-law illuminates a relativistic accretion disc and produces a reflection spectrum (see Sect. 2.3.2) which includes a Compton ‘hump’ at about 30 keV, a strong fluorescent Fe K$\alpha$ line at 6.4 keV, and a soft X-ray excess, composed of many emission lines that are blurred by relativistic motion in the accretion disc. \cite{Crummy_2006} have reported that the reflection model makes a bet-
ter fit to the EPIC-pn spectra of 22 Type-1 PG quasars and 12 Seyfert-1 galaxies than the conventional model of power-law and blackbody. However, no optical/UV data are fitted in [Crummy et al. (2006)] and so their reflection modelling is not tested at a broad-band level. Furthermore, fitting the soft X-ray excess using this reflection model requires fine-tuning of the ionisation parameter and inclination angle of the disc, and almost maximally rotating black holes for all the objects. [Done and Nayakshin (2007)] have explored further the disc reflection model to check whether it can account for the soft X-ray excess in AGN, using the additional constraint of hydrostatic balance on the structure of the illuminated disc atmosphere. They conclude that reflection from a hydrostatic disc cannot produce the soft X-ray excess, and constant density disc models require fine-tuning and suppression of the intrinsic continuum to produce the largest observed soft excesses.

For the case of Mrk 509, I found that the significantly variable part of the X-ray continuum is the soft excess component, which is strongly correlated with the variability of the optical/UV disc emission. The hard X-ray power-law displays smaller variability than the soft excess and seems unconnected to the other spectral components over the probed timescales. The reflection spectrum is produced as a result of the illumination of the disc by the power-law and the blurred reflection component is generally expected to be less variable than the power-law. Thus it is unlikely that in Mrk 509 the observed soft X-ray excess, which varies in a very similar fashion to the disc intrinsic emission, is caused by reflection over the probed timescales.

The more likely possibility for the origin of the soft X-ray excess in Mrk 509 is up-scattering of the disc photons in a warm Comptonising corona with lower temperature and higher optical depth than the one responsible for the X-ray power-law (i.e. the hot corona). From broad-band spectral analysis of the Seyfert-1 NGC 5548, [Magdziarz et al. (1998)] have found that the soft excess requires a separate continuum component which can be fitted by Comptonisation of thermal photons from a cold disc \( (T_{\text{max}} \sim 3.2 \text{ eV}) \), in a warm \( (\sim 0.3 \text{ keV}) \), optically thick \( (\tau \sim 30) \) plasma. The authors also find the optical/UV and soft X-ray fluxes in NGC 5548 to be closely correlated. Their results are similar to what I have found for Mrk 509. [Middleton et al. (2009)] and [Jin et al. (2009)] also report that the soft X-ray excess in the NLSy1s RE J1034+396 and RX J0136.9–3510 can be explained as the result of
warm Comptonisation of the disc emission. Furthermore, Done and Kubota (2006) have shown that an optically-thick Comptonising corona over the inner regions of the disc in some Black Hole Binaries (BHBs, e.g. XTE J1550–564) can distort a standard disc spectrum to produce a strong, steep tail extending to higher energies (shown in Figs. 4 and 5 of Done and Kubota 2006); this is seen in the Very High State of BHBs, when the X-ray spectra show both a strong disc component and a strong high-energy tail (although in this state of BHBs the hard X-ray power-law seems to be usually absent). This high-energy tail in the Very High State of BHBs may be analogous in nature (although the temperature of the Comptonised gas is substantially higher) to the tail of the warm Comptonisation which appears as a soft excess in the X-ray spectra of Seyferts like Mrk 509. Also, Zdziarski et al. (2001) have fitted the spectrum of the BHB GRS 1915+105 in the Gamma-Ray State, by warm Comptonisation of the disc blackbody in a plasma with a temperature of 3.6 keV and an optical depth of 4.4 (see their Fig. 3b).

My broad-band variability study of Mrk 509 has shown the existence of a strong link between the disc emission and the soft X-ray excess, suggesting that the disc photons are up-scattered in a warm Comptonising corona close to the inner disc, with a temperature of about 0.2 keV and an optical depth of about 17 (see Table 6.8). The scattered fraction of the original disc photons by the corona is $C_f[1 - \exp(-\tau)]$, where $C_f$ is the covering fraction of the corona over the disc and $\tau$ is the optical depth of the corona; this estimation neglects any angle dependencies of the seed and scattered photons. From the broad-band modelling described in Sect. 6.5 the number of disc photons and the disc luminosity before and after scattering by the corona are obtained using the disc and Comptonisation emission components. Thus the fraction of scattered disc photons by the corona and hence the corona covering fraction $C_f$ and also the fraction of accretion disc power dissipated into the corona can be calculated. For Mrk 509, $C_f$ of the warm corona is estimated to be about 0.25 and the fraction of disc power dissipated into the warm corona is calculated to be also about 0.25.

6.6.3 Black hole mass and accretion rate in Mrk 509

From the disc blackbody fits one can estimate the accretion rate $\dot{M}$ for Mrk 509 using the normalisation area $A = R_{in}^2 \cos i$ and the temperature $T_* = [3GM\dot{M}/(8\pi R_{in}^3 \sigma)]^{1/4}$. To do this the mass of the black hole is required.
Peterson et al. (2004) have calculated the black hole mass $M$ of 35 AGN from previously published broad line reverberation-mapping data: $M = f c \tau_{\text{cent}} \sigma_{\text{line}}^2 / G$,
where $f = 5.5$ is a scaling factor, $\tau_{\text{cent}}$ is the emission line time lag relative to the continuum, characterised by the centroid of the cross correlation function, $\sigma_{\text{line}}$ is the width of the emission line, $c$ the speed of light and $G$ the gravitational constant. For Mrk 509 the black hole mass is reported to be $1.43 \times 10^8 \, M_\odot$. However, here I re-calculate the black hole mass using $\tau_{\text{cent}}$ as measured by Carone et al. (1996): this is a paper entirely dedicated to the determination of $\tau_{\text{cent}}$ for the case of Mrk 509 where $\tau_{\text{cent}}$ is found to be 80.2 days for the H$\beta$ line. The H$\beta$ line width which I measured from the OM grism spectrum (Table 6.5) is also used: $\sigma_{\text{line}} = \text{FWHM} / \sqrt{\ln 256} = 1869 \, \text{km s}^{-1}$. Adopting these values I calculate a black hole mass of $3.0 \times 10^8 \, M_\odot$ for Mrk 509, which is twice as large as the value reported in Peterson et al. (2004). So, for this mass and a Schwarzschild geometry black hole, from the normalisation $A$ and temperature $T_*$, one finds $\dot{M}$ has a range of 0.24 to 0.34 $M_\odot \, \text{y}^{-1}$ during the XMM-Newton campaign. Assuming a reasonable inclination angle $i$ of $30^\circ$ to $45^\circ$, a range of 6.0 to 7.0 $R_g$ for the inner-disc radius $R_{\text{in}}$ is obtained.
Chapter 7

ESO 113-G010: ionised outflows and nuclear obscuration

This chapter is based on Mehdiipour et al. (2012), A&A, 542, A30.

In this chapter I present the first-ever analysis of the X-ray warm absorber and nuclear obscuration in the Seyfert 1.8 galaxy ESO 113-G010. Archival data from a 100 ks XMM-Newton observation made in 2005 are used. From high-resolution X-ray spectroscopy analysis of the RGS data, I detect absorption lines originating from a warm absorber consisting of two distinct phases of ionisation, with \( \log \xi \approx 3.2 \) and 2.3 respectively. The higher-ionised component has a larger column density and outflow velocity \( (N_H \approx 1.6 \times 10^{22} \text{ cm}^{-2}, v \approx -1100 \text{ km s}^{-1}) \) than the lower-ionised component \( (N_H \approx 0.5 \times 10^{22} \text{ cm}^{-2}, v \approx -700 \text{ km s}^{-1}) \). The shape of the optical/UV continuum and the large Balmer decrement \( (\text{H} \alpha / \text{H} \beta \sim 8) \) indicate significant amount of reddening is taking place in our line of sight in the host galaxy of the AGN; however, the X-ray spectrum is not absorbed by cold neutral gas intrinsic to the source. I discuss different explanations for this discrepancy between the reddening and the X-ray absorption, and suggest that the most likely solution is a dusty warm absorber. I show that dust can exist in the lower-ionised phase of the warm absorber and cause the observed reddening of the optical/UV emission, whereas the X-rays remain unabsorbed due to lack of cold neutral gas in the ionised warm absorber. Furthermore, I have investigated the uncertainties in the construction of the SED of this object due to obscuration of the nuclear source and the effects these have on the photoionisation modelling of the warm absorber.
I show how the assumed SEDs influence the thermal stability of each phase and whether or not the two absorber phases in ESO 113-G010 can co-exist in pressure equilibrium.

7.1 Introduction

ESO 113-G010 was first identified and catalogued as a galaxy (SBa) in the ESO/Uppsala Survey of the ESO(B) Atlas (Lauberts 1982), based on observations made with the ESO 1 m Schmidt telescope at La Silla, Chile. From its first-ever X-ray observation with ROSAT in 1995 and follow-up optical spectroscopy in 1996 with the 2.2 m ESO/MPG telescope at La Silla observatory, Pietsch et al. (1998) have classified it as a Seyfert 1.8 galaxy at a redshift of 0.025701.

The next time ESO 113-G010 was observed in the X-rays was with XMM-Newton in May 2001. From spectral analysis of the 4 ks EPIC-pn data, Porquet et al. (2004) reported the presence of a soft X-ray excess and a highly redshifted Fe Kα line at 5.4 keV. The only other X-ray observation of ESO 113-G010 to this date was 100 ks long and performed with XMM-Newton in November 2005. Porquet et al. (2007) reported strong rapid variability from their power spectral density timing analysis of the EPIC-pn data. Furthermore, from spectral analysis of the iron line band, no redshifted Fe Kα line was detected, contrary to the 2001 findings, while the presence of two narrow emission lines at about 6.5 keV and 7 keV was reported.

In this work I present the first analysis of the RGS spectra from the 100 ks XMM-Newton observation of 2005, which show clear signs of warm absorber outflows. I also used the simultaneous EPIC-pn and OM data to aid the photoionisation modelling of the outflows. Some details of the XMM-Newton observations of ESO 113-G010 are shown in Table 7.1. The structure of this chapter is as follows. Section 7.2 describes the nuclear obscuration of the AGN. Spectral analysis and photoionisation modelling of the warm absorber are described in Sect. 7.3. Construction of the SEDs and modelling with different SEDs are described in Sect. 7.4 and my findings are discussed in Sect. 7.5. My conclusions and implications of this work are given in Chapter 8.

Note that all the spectra and SEDs in this chapter are displayed in the observed frame. The RGS spectra shown are background-subtracted.
7.2 Intrinsic obscuration of the nuclear source

7.2.1 Nuclear obscuration from the Balmer decrement

ESO 113-G010 is classified as a Seyfert 1.8 galaxy by Pietsch et al. (1998), following the Osterbrock (1981) observational classification of Seyfert-1 AGN (see Sect. 1.3.1). The Hα/Hβ line ratio is not one of the properties given in Pietsch et al. (1998), so I re-analysed their optical spectrum (shown in Fig. 7.1) in order to obtain the Balmer decrement. Both the Hα λ6563 and Hβ λ4861 lines were fitted with two narrow and broad Gaussian-profile components. The two forbidden lines of [N ii] λλ6548, 6583, which are blended with Hα, were also modelled with narrow Gaussian-profile components. To calculate the Hα/Hβ ratio the total flux of each line (including both narrow and broad components) were used, since the broad component of Hβ is very weak and de-blending of the narrow and broad components of the lines increases the uncertainty in the flux measurements. So the Balmer decrement and consequently the reddening calculated here are averages over the NLR and BLR. The observed Balmer decrement is found to be Hα/Hβ = 7.96. The FWHM is about 2000 km s⁻¹ for the broad components and about 500 km s⁻¹ for the narrow components of the above lines.

To convert the Balmer decrement into reddening $E(B-V)$, the mean extinction curve of Gaskell and Benker (2007), obtained with HST for a sample of AGN, was used. Their best determined extinction curves are flatter in the far-UV and are missing the λ2175 bump compared to the standard Galactic curve (see e.g. Cardelli et al. 1989; Osterbrock 1989). The relationship $f_{\lambda, \text{obs}} = f_{\lambda, \text{int}} 10^{-0.4 A_\lambda}$ gives

$$\log \left( \frac{R_{\text{obs}}}{R_{\text{int}}} \right) = -0.4 \left( A_{\lambda, \text{H} \alpha} - A_{\lambda, \text{H} \beta} \right)$$

where $R_{\text{obs}}$ and $R_{\text{int}}$ are the observed and intrinsic Balmer decrements Hα/Hβ; $A_{\lambda, \text{H} \alpha}$ and $A_{\lambda, \text{H} \beta}$ represent the extinction at the wavelengths of the Balmer lines. Using the parameterisation of the mean extinction curve of Gaskell and Benker (2007),
7.2. Intrinsic obscuration of the nuclear source

\[ \lambda (\mathring{A}) \]

Fig. 7.1: The optical spectrum of the Seyfert 1.8 galaxy ESO 113-G010 taken from Pietsch et al. (1998). Flux density \( F_\lambda \) in units of \( 10^{-15} \text{ erg cm}^{-2} \text{ s}^{-1} \mathring{A}^{-1} \) is plotted versus the observed wavelength \( \lambda \).

one obtains the colour excess

\[ E(B-V) = 1.790 \log \left( \frac{R_{\text{obs}}}{R_{\text{int}}} \right) \]  

(7.2)

The scalar specifying the ratio of total to selective extinction \( R_V \equiv A_V/E(B-V) \) was fixed at 3.1.

From theoretical recombination studies, the Balmer decrement \( \text{H}_\alpha/\text{H}_\beta = 2.85 \) for Case B recombination at a temperature \( T = 10^4 \text{ K} \) and electron density \( n_e = 10^4 \text{ cm}^{-3} \) (Osterbrock and Ferland 2006). Case B refers to the recombination which takes place in a typical nebula with a large enough optical depth that Lyman-line photons are scattered \( n \) times and are converted (if \( n \geq 3 \)) into lower-series photons plus either Ly-\( \alpha \) or two-continuum photons, so that they cannot escape from the nebula (Osterbrock and Ferland 2006). For the NLR and BLR of AGN, which have higher electron density than a nebula, this value requires modification due to contribution to the \( \text{H}_\alpha \) line from collisional excitation. For the NLR of AGN the intrinsic Balmer decrement \( \text{H}_\alpha/\text{H}_\beta \) is about 3.1 (Osterbrock and Ferland 2006). This value however may be different for the BLR as clouds have higher density in this region. Ferguson and Ferland (1997) have computed the ratio of Balmer lines relative to \( \text{H}_\beta \) for realistic conditions in BLR clouds. For a BLR with \( T = 10^4 \text{ K} \) and \( n_e = 10^{11} \text{ cm}^{-3} \), they obtain an intrinsic \( \text{H}_\alpha/\text{H}_\beta = 3.28 \).
From observations, Ward et al. (1988) have measured the average intrinsic H_α/H_β in BLR to be 3.5, independent of any atomic physics assumptions. Using a similar approach, Carrera et al. (2004) have also measured the intrinsic H_α/H_β to be 3.43. So in my calculations I take $R_{\text{int}} = 3.1 - 3.5$ and $R_{\text{obs}}$ to be 7.96, which yields intrinsic $E(B-V) = 0.64 - 0.73$. The extinction curve of Gaskell and Benker (2007) was then used to correct all the optical/UV data for reddening in the host galaxy of the AGN, using $E(B-V) = 0.64 - 0.73$.

### 7.2.2 Nuclear obscuration from the optical/UV continuum

Intrinsic reddening will also affect the optical/UV continuum and change the shape of the big-blue-bump, which is attributed to thermal emission from the accretion disc (see Sect. 2.1). The optical/UV continuum in ESO 113-G010 is AGN-dominated; for the purpose of my study contaminating emission by the stars in the host galaxy would have a negligible effect on the SED and photoionisation modelling. I corrected the continuum in such a way that (1) the optical slope ($\alpha_{\text{opt}}$) and (2) the relation between optical-to-X-ray spectral index ($\alpha_{\text{ox}}$) and the log_{10} of the monochromatic optical luminosity at 2500 Å ($l_{\text{opt}}$) are consistent with AGN samples found in surveys.

Young et al. (2010) have cross-correlated the Sloan Digital Sky Survey (SDSS) DR5 quasar catalog with the XMM-Newton archive, and have obtained $\alpha_{\text{opt}}$ and $\alpha_{\text{ox}}$ for a sample of 327 quasars with high X-ray signal-to-noise ratio, where both optical and X-ray spectra are available. Young et al. (2010) find $\alpha_{\text{opt}} = -0.40$, which is also similar to the slope $\alpha_{\text{opt}} = -0.44$ found by Vanden Berk et al. (2001) for mean composite quasar spectra using a dataset of over 2200 spectra from the SDSS.

For the uncorrected continuum of ESO 113-G010, $\alpha_{\text{opt}} = -1.74$, which indicates reddening. So the extinction curve of Gaskell and Benker (2007) was used to correct the optical/UV data for reddening to match the $\alpha_{\text{opt}} = -0.40$. It is found that the amount of reddening required for this correction corresponds to $E(B-V) = 0.39$, which is less than $E(B-V)$ range of 0.64 to 0.73, inferred from the Balmer decrement.

Furthermore, my values of $\alpha_{\text{ox}}$ and $l_{\text{opt}}$ were checked against the $\alpha_{\text{ox}}$-$l_{\text{opt}}$ relation found by Young et al. (2010). As shown in Table 7.2, for the uncorrected (not de-reddened) case and the de-reddened case using the optical/UV continuum, the $\alpha_{\text{ox}}$ values are consistent within the dispersion in the $\alpha_{\text{ox}}$-$l_{\text{opt}}$ relation of Young et al.
7.2. Intrinsic obscuration of the nuclear source

<table>
<thead>
<tr>
<th></th>
<th>Not de-reddened</th>
<th>De-reddened using the Balmer decrement</th>
<th>De-reddened using the optical/UV continuum</th>
</tr>
</thead>
<tbody>
<tr>
<td>log $l_{\text{opt}}$</td>
<td>28.0</td>
<td>29.7 to 29.9</td>
<td>29.1</td>
</tr>
<tr>
<td>$\alpha_{\text{ox}}$</td>
<td>−1.2</td>
<td>−2.0 to −1.9</td>
<td>−1.6</td>
</tr>
<tr>
<td>Young et al. (2010)</td>
<td>$\alpha_{\text{ox}}$</td>
<td>−1.4 to −1.1</td>
<td>−1.6 to −1.3</td>
</tr>
</tbody>
</table>

* $\log_{10}$ of the monochromatic optical luminosity of ESO 113-G010 at 2500 Å in erg s$^{-1}$ Hz$^{-1}$.
* The optical-to-X-ray spectral index of ESO 113-G010.
* The optical-to-X-ray spectral index from the Young et al. (2010) $\alpha_{\text{ox}}$-$l_{\text{opt}}$ relation for AGN.

On the other hand, for the de-reddened case using the Balmer decrement, $\alpha_{\text{ox}}$ is not consistent with the $\alpha_{\text{ox}}$ from the Young et al. (2010) relation for the corresponding log $l_{\text{opt}}$. This may indicate that the Balmer decrement over-estimates the amount of reddening; I return to this issue in Sect. 7.5.1.

7.2.3 Intrinsic X-ray obscuration of the nuclear source by cold gas?

From the intrinsic reddening $E(B-V)$ values calculated in Sect. 7.2.1 from the Balmer decrement and in Sect. 7.2.2 based on the continuum reddening, the associated column density of cold gas in ESO 113-G010 can be estimated. The relationship between hydrogen column density $N_{\text{H}}$ and optical extinction $A_V$ can be written as $N_{\text{H}}$ (cm$^{-2}$) = $a \times 10^{21} A_V$ (mag), where the factor $a$ is reported to be 2.22 in Gorenstein (1975), 1.79 in Predehl and Schmitt (1993), 1.89 in Osterbrock and Ferland (2006) and 2.21 in Güver and Özel (2009). Therefore, one can calculate a range of values for $N_{\text{H}}$ using the different values of $E(B-V)$ and $a$ given above. This gives $N_{\text{H}} = (3.5–5.0) \times 10^{21}$ cm$^{-2}$ if using $E(B-V)$ calculated from the Balmer decrement and $N_{\text{H}} = (2.2–2.7) \times 10^{21}$ cm$^{-2}$ if using $E(B-V)$ calculated from the continuum reddening.

However, analyses of the X-ray spectra show that ESO 113-G010 is not intrinsically absorbed by a large column of neutral gas. Porquet et al. (2004) obtain an upper limit of $8 \times 10^{19}$ cm$^{-2}$ to intrinsic absorption from analysis of the 2001 EPIC-pn spectrum. This is indeed much lower than the predicted values of $(3.5–5.0) \times 10^{21}$ cm$^{-2}$ or $(2.2–2.7) \times 10^{21}$ cm$^{-2}$ calculated above from the intrinsic reddening.
Porquet et al. (2007) also mention that during the 2005 XMM-Newton observation, instead of intrinsic neutral absorption expected below about 1 keV, a soft X-ray excess is observed. From analysis of the 2005 EPIC-pn spectrum, I obtain an upper limit of $8.9 \times 10^{19} \text{ cm}^{-2}$ (at 99% confidence level) to the column density $N_{\text{H}}$ of intrinsic neutral gas. This upper limit is compatible with that found by Porquet et al. (2004) for the 2001 data. This apparent discrepancy between the optical/UV reddening and X-ray absorption, and its implications, are discussed in Sect. 7.5.1.

### 7.3 Photoionisation modelling and spectral analysis of the warm absorber

I began modelling the soft X-ray spectrum of ESO 113-G010 by fitting the RGS continuum with a cosmologically redshifted power-law. In all the fits the effects of the Galactic neutral absorption were included by applying the hot model (introduced in Sect. 3.4) in spex. Assuming Lodders et al. (2009) abundances, the Galactic H\(_{\text{i}}\) column density in our line of sight was fixed at $N_{\text{H}} = 2.78 \times 10^{20} \text{ cm}^{-2}$ (Dickey and Lockman 1990) and the gas temperature of the hot model at 0.5 eV to mimic a neutral gas in collisional ionisation equilibrium. I also tested the more recent tbnew model (Wilms et al. in prep) which describes X-ray absorption in the ISM using the Wilms et al. (2000) abundances within the xspec package (Arnaud 1996). The features in the vicinity of the K-edges of Ne and O and the L-edge of Fe are found to be very similar in both the tbnew and hot models as shown in Fig. 7.2. Therefore, using the tbnew model would not change the results of my study. Furthermore, I checked the impact of using the slightly smaller $N_{\text{H}}$ value of $2.08 \times 10^{20} \text{ cm}^{-2}$ from the Leiden/Argentine/Bonn (LAB) Survey of Galactic H\(_{\text{i}}\) (Kalberla et al. 2005) on my analysis and found that all parameters derived in this work remain unchanged within the given errors.

The power-law fit, letting photon index and normalisation free, led to a $\chi^2/\nu$ value of 1.6 (1054 d.o.f.). The fit was not satisfactory as there were absorption features which were not fitted by the Galactic absorption model. At this stage one xabs component (see Sect. 3.4) was included in the model. For an assumed SED of the source, the ionisation balance calculations (see Sect. 3.1) were performed using version C08.00 of cloudy (Ferland et al. 1998) with Lodders et al. (2009) abundances. I made runs with cloudy for a grid of ionisation parameter $\xi$ values (log $\xi$
7.3. Photoionisation modelling and spectral analysis of the warm absorber

Fig. 7.2: The tbnew and hot ISM X-ray absorption models, as described in Sect. 7.3, were applied to the power-law continuum of ESO 113-G010 and are shown in the vicinity of the K-edges of Ne (left panels) and O (right panels) and the L-edge of Fe (middle panels).

between −8.5 and +6.5 with steps of 0.1) in order to calculate the equilibrium ion concentrations. As a start, the SED of the Seyfert-1 galaxy Mrk 509 (Kaastra et al. 2011a) was adopted (but see Sect. 7.4 for detailed modelling with different SEDs for ESO 113-G010). This SED was established with the help of simultaneous data from a large multi-wavelength campaign, and broad-band modelling of the underlying continuum (see also Chapter 6), and is likely to be representative of the real SED shape for a typical Seyfert galaxy (SED G in Fig. 7.5). In my modelling, the ionisation parameter ($\xi$), the equivalent hydrogen column density ($N_H$) of the warm absorber, its flow and RMS velocities were fitted. The inclusion of the xabs component improved $\chi^2$ to 1.22 (1050 d.o.f.). There were, however, absorption lines in the lower energy part of the spectrum which could not be fitted with a single xabs phase, since they are less highly ionised and have a different velocity. So a second xabs phase was introduced in the model to obtain a better fit to the data. The addition of this second phase further improved $\chi^2$ to 1.12 (1046 d.o.f.) and all the significantly detected absorption features were fitted. I tested adding another xabs component, but this did not make the fit any better, so two xabs components are deemed to be sufficient to model the warm absorption in ESO 113-G010. Finally, the above analysis was repeated using other SEDs adopted for ESO 113-G010, which are described in Sec. 7.4 and shown in Fig. 7.5.
7.3. Photoionisation modelling and spectral analysis of the warm absorber

Fig. 7.3: Top panel: RGS spectrum of ESO 113-G010, fitted using the two-phase $x_{\text{abs}}$ model described in Sect. 7.3 and SED E in Fig. 7.3. The data are shown in red and the best-fit model in blue. Residuals of the fit, $(\text{Observed} - \text{Model})/\text{Model}$, are displayed below the panel. Bottom panel: The absorption components of the RGS model described in Sect. 7.3 with the best-fit parameters given in Table 7.3. The blue component shows the Galactic absorption applied to the power-law continuum (in black). The two warm absorber phases (phase 1 in red and phase 2 in green) are applied separately to the Galactic-absorbed continuum, showing how each phase contributes to the absorption.
Fig. 7.4: Close-ups of the parts of the RGS spectrum and the best-fit model (from the two-phase $x_{\text{abs}}$ modelling described in Sect. 7.3 and using SED E in Fig. 7.5) where the most prominent absorption lines are detected. The data are shown in red and the model in blue. Residuals of the fit, $(\text{Observed} - \text{Model})/\text{Model}$, are displayed below each panel. 

*Figure continued next page.*
7.3. Photoionisation modelling and spectral analysis of the warm absorber

Fig. 7.4: Continued from previous page.

Table 7.3: Best-fit parameters of the power-law continuum and two-phase warm absorber xabs model of ESO 113-G010, obtained from fitting the RGS spectrum as described in Sect. and using SED E in Fig. (\(\chi^2 = 1.12\) for 1046 d.o.f.). The fitted parameter errors are quoted at 90% confidence for one interesting parameter.

<table>
<thead>
<tr>
<th></th>
<th>(\Gamma^a)</th>
<th>(\text{Norm}^b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power-law:</td>
<td>2.62 ± 0.05</td>
<td>3.1 ± 0.1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>xabs</th>
<th>(\log \xi^c)</th>
<th>(N_H^d)</th>
<th>Flow (\nu^e)</th>
<th>RMS (\nu^e)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phase 1:</td>
<td>3.2 ± 0.1</td>
<td>1.6 ± 1.0</td>
<td>−1100 ± 300</td>
<td>500 ± 300</td>
</tr>
<tr>
<td>Phase 2:</td>
<td>2.3 ± 0.1</td>
<td>0.5 ± 0.2</td>
<td>−700 ± 100</td>
<td>100 ± 40</td>
</tr>
</tbody>
</table>

\(a\) Photon index.
\(b\) Normalisation in \(10^{51}\) photons s\(^{-1}\) keV\(^{-1}\) at 1 keV.
\(c\) \(\text{erg cm s}^{-1}\).
\(d\) \(10^{22}\) cm\(^{-2}\).
\(e\) km s\(^{-1}\).
Table 7.4: Total column densities of the most relevant ions of the warm absorber outflow in ESO 113-G010, derived from the \texttt{xabs} modelling described in Sect. 7.3. Percentages of ionic column density produced by each warm absorber phase are also shown. The ranges of values given correspond to the minimum and maximum values found using the different SEDs of Fig. 7.5.

<table>
<thead>
<tr>
<th>ion</th>
<th>log $N_{\text{ion}}$ (cm$^{-2}$)</th>
<th>Phase 1</th>
<th>Phase 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>H I</td>
<td>13.33 - 15.30</td>
<td>3.22 - 5.76</td>
<td>94.24 - 96.78</td>
</tr>
<tr>
<td>H II</td>
<td>22.26 - 22.32</td>
<td>75.71 - 79.62</td>
<td>20.38 - 24.29</td>
</tr>
<tr>
<td>C VI</td>
<td>17.09 - 17.15</td>
<td>7.25 - 9.87</td>
<td>90.13 - 92.75</td>
</tr>
<tr>
<td>N VII</td>
<td>16.97 - 17.02</td>
<td>9.03 - 11.86</td>
<td>88.14 - 90.97</td>
</tr>
<tr>
<td>O VII</td>
<td>17.28 - 17.35</td>
<td>0.54 - 0.75</td>
<td>99.25 - 99.46</td>
</tr>
<tr>
<td>O VIII</td>
<td>18.11 - 18.16</td>
<td>13.28 - 16.95</td>
<td>83.05 - 86.72</td>
</tr>
<tr>
<td>Ne IX</td>
<td>17.39 - 17.42</td>
<td>2.02 - 2.73</td>
<td>97.27 - 97.98</td>
</tr>
<tr>
<td>Ne X</td>
<td>17.63 - 17.66</td>
<td>42.76 - 49.58</td>
<td>50.42 - 57.24</td>
</tr>
<tr>
<td>Mg XI</td>
<td>17.11 - 17.14</td>
<td>12.59 - 17.93</td>
<td>82.07 - 87.41</td>
</tr>
<tr>
<td>Mg XII</td>
<td>17.29 - 17.30</td>
<td>84.97 - 88.58</td>
<td>11.42 - 15.03</td>
</tr>
<tr>
<td>Si X</td>
<td>16.53 - 16.55</td>
<td>0.00 - 0.01</td>
<td>99.99 - 100.00</td>
</tr>
<tr>
<td>Si XI</td>
<td>16.55 - 16.58</td>
<td>0.06 - 0.18</td>
<td>99.82 - 99.94</td>
</tr>
<tr>
<td>Si XII</td>
<td>16.45 - 16.50</td>
<td>3.23 - 6.25</td>
<td>93.75 - 96.77</td>
</tr>
<tr>
<td>Si XIII</td>
<td>17.13 - 17.18</td>
<td>61.58 - 70.93</td>
<td>29.07 - 38.42</td>
</tr>
<tr>
<td>Si XIV</td>
<td>17.40 - 17.46</td>
<td>98.12 - 98.88</td>
<td>1.12 - 1.88</td>
</tr>
<tr>
<td>S XII</td>
<td>16.37 - 16.43</td>
<td>0.04 - 0.18</td>
<td>99.82 - 99.96</td>
</tr>
<tr>
<td>S XIII</td>
<td>15.99 - 16.08</td>
<td>2.09 - 4.61</td>
<td>95.39 - 97.91</td>
</tr>
<tr>
<td>S XIV</td>
<td>15.79 - 15.93</td>
<td>51.73 - 66.12</td>
<td>33.88 - 48.27</td>
</tr>
<tr>
<td>S XV</td>
<td>16.94 - 17.01</td>
<td>97.17 - 98.30</td>
<td>1.70 - 2.83</td>
</tr>
<tr>
<td>S XVI</td>
<td>16.96 - 17.08</td>
<td>99.90 - 99.95</td>
<td>0.05 - 0.10</td>
</tr>
<tr>
<td>Fe XVII</td>
<td>16.62 - 16.71</td>
<td>2.84 - 10.41</td>
<td>89.59 - 97.16</td>
</tr>
<tr>
<td>Fe XVIII</td>
<td>16.56 - 16.64</td>
<td>35.55 - 50.92</td>
<td>49.08 - 64.45</td>
</tr>
<tr>
<td>Fe XIX</td>
<td>16.81 - 16.85</td>
<td>91.08 - 94.10</td>
<td>5.90 - 8.92</td>
</tr>
<tr>
<td>Fe XX</td>
<td>17.05 - 17.10</td>
<td>99.66 - 99.80</td>
<td>0.20 - 0.34</td>
</tr>
<tr>
<td>Fe XXI</td>
<td>17.10 - 17.13</td>
<td>99.99 - 99.99</td>
<td>0.01 - 0.01</td>
</tr>
<tr>
<td>Fe XXII</td>
<td>16.83 - 16.96</td>
<td>100.00 - 100.00</td>
<td>0.00 - 0.00</td>
</tr>
<tr>
<td>Fe XXIII</td>
<td>16.42 - 16.71</td>
<td>100.00 - 100.00</td>
<td>0.00 - 0.00</td>
</tr>
</tbody>
</table>
In the top panel of Fig. 7.3, the RGS spectrum and the best-fit model are presented and in the bottom panel it is shown how each phase in the model contributes to the absorption. In Fig. 7.4, close-ups of the parts of the RGS spectrum where the most prominent absorption lines are detected are shown. The best-fit parameters of the model (obtained using SED E in Fig. 7.5 – see also Sect. 7.4.4) are shown in Table 7.3. Note that the best-fit velocities of the warm absorber phases are found to be the same for the different SEDs of Fig. 7.5. Furthermore, the only parameter of the warm absorber outflows which significantly changes as a consequence of using different SEDs is the ionisation parameter $\xi$, whose values are given in Fig. 7.6. The total column densities of different ions in the two warm absorber phases are listed in Table 7.4.

7.4 Modelling with different Spectral Energy Distributions

In order to calculate a more accurate ionisation balance required to improve the photoionisation modelling of the warm absorber, it is essential to determine the broad-band continuum of the source. Note that there are few flux measurements for ESO 113-G010 compared to some of the well-studied Seyfert galaxies. In the following subsections I describe how different parts of the SED were constructed. Then in Sect. 7.4.4 I discuss the uncertainties in the construction of the SED due to nuclear obscuration of the source and how, in order to investigate the effects of these uncertainties, different SEDs were selected for further modelling.

7.4.1 Interstellar de-reddening in our Galaxy

All the optical/UV fluxes were corrected for interstellar reddening in our Galaxy using the reddening curve of Cardelli et al. (1989), including the update for near-UV given by O'Donnell (1994). The Galactic interstellar colour excess $E(B - V) = 0.025$ mag is based on calculations of Schlegel et al. (1998) as shown in NED. Also in this case $R_V$ was fixed at 3.1.

7.4.2 Optical/IR/radio part of the SED

Optical flux measurements in Cousin’s $B$ (440 nm) and $R$ (640 nm) bands were taken from the Surface Photometry Catalogue of the ESO-Uppsala Galaxies (Lauberts and Valentijn, 1989). Infrared flux measurements were extracted at $J$
(1.25 \mu m), H (1.65 \mu m) and K_S (2.17 \mu m) bands from the 2MASS All-Sky Catalog of Point Sources (Cutri et al. 2003). Furthermore, I used far-IR data at 12 \mu m, 25 \mu m, 60 \mu m and 100 \mu m from the IRAS Faint Source Catalog (Moshir et al. 1990), and at 160 \mu m from the AKARI/FIS All-Sky Survey Bright Source Catalog (Yamamura et al. 2010). These data points are shown as circles in the SEDs displayed in Fig. 7.5; the red circles are for fluxes corrected only for Galactic extinction as described in Sect. 7.4.1 (SEDS A and B), whereas the fluxes shown as blue circles are also corrected for extinction in the host galaxy of the AGN as described in Sects. 7.2.1 (Balmer decrement, SEDs C and D) and 7.2.2 (optical/UV continuum, SEDs E and F). Note that the fluxes used here are AGN-dominated but include some stellar optical emission coming from the nuclear region of the galaxy and IR dust emission from the whole galaxy; however, for the purpose of this study, contaminating emission by the host galaxy would have a negligible effect on the broad-band SED and photoionisation modelling.

The only radio-band flux measurement available for ESO 113-G010 was found in the Sydney University Molonglo Sky Survey (SUMSS) Source Catalog (Mauch et al. 2003). The flux at 36 cm (outside the plots in Fig. 7.5) is 13.9 \pm 1.0 mJy.

7.4.3 UV/X-ray part of the SED

The UV part of the SED was constructed from the XMM-Newton OM observation and the GALEX All-sky Imaging Survey (AIS). The 2005 OM data were taken in the \textit{U} (3440 \AA), \textit{UVW1} (2910 \AA), \textit{UVM2} (2310 \AA) and \textit{UVW2} (2120 \AA) filters. The 2007 GALEX data were taken in the NUV (2267 \AA) and FUV (1516 \AA) filters. Note that the OM UV data (which are simultaneous with the X-rays) are not simultaneous with the GALEX UV data. However, the OM \textit{UVM2} flux is consistent with the GALEX NUV flux, which indicates that the UV flux was at a similar level during the XMM-Newton and GALEX observations. The OM and GALEX data are shown as squares in the SEDs displayed in Fig. 7.5; the red squares show fluxes corrected only for Galactic extinction as described in Sect. 7.4.1 whereas the blue squares are for fluxes also corrected for extinction in the host galaxy of the AGN as described in Sects. 7.2.1 (SEDS C and D) and 7.2.2 (SEDS E and F).

The 0.3–10 keV X-ray part of the SED was constructed using the EPIC-pn data, corrected for the Galactic H\textsubscript{1} column density in our line of sight, $N_H = 2.78 \times 10^{20} \text{ cm}^{-2}$, given by Dickey and Lockman (1990). The EPIC-pn data are
shown as small green circles in the SEDs displayed in Fig. 7.5. Unfortunately, there are no X-ray data available for ESO 113-G010 above 10 keV; therefore in order to estimate the SED above 10 keV, the high energy part of the EPIC-pn spectrum was extrapolated using a power-law model up to 20 keV \((4.84 \times 10^{18} \text{ Hz})\); then from 20 keV to 162 keV, the INTEGRAL data from the SED of Mrk 509 as given in Kaastra et al. (2011a) were used, but scaled down to match the ESO 113-G010 flux at 20 keV. This way the shape of the ESO 113-G010 SED above 10 keV resembles the Compton hump (Sect. 2.3.2) commonly seen in Seyfert AGN. I have tested whether the shape of the continuum above 10 keV, and in particular the shape and flux of the Compton hump, affect the results of the warm absorber analysis and the thermal stability curves (Sect. 7.4.3); it is found that changing the hard X-ray continuum does not modify my results significantly and the derived parameters remain unchanged within the given errors.

7.4.4 Different assumed SEDs for modelling

Different SEDs of the ionising source can have a significant effect on the ionisation balance of the absorbing material and consequently affect the stability and structure of the warm absorber. So I have taken into account the uncertainties by adopting different SEDs in my further modelling of the warm absorber.

For the case of ESO 113-G010, the largest uncertainty arises from the level of extinction and reddening in the host galaxy of the AGN, reported in Sect. 7.2: (1) there is uncertainty in measuring the Balmer decrement in ESO 113-G010 and (2) the Balmer decrement can be intrinsic to the BLR or NLR clouds, so there are uncertainties in deriving reddening information from the Balmer decrement. As shown in Fig. 7.5, I considered SEDs corrected only for Galactic extinction (SEDs A, B), and with also the AGN obscuration taken into account as described in Sect. 7.2.1 (SEDs C, D), based on the Balmer decrement, and Sects. 7.2.2 (SEDs E, F), based on the continuum reddening. Furthermore, the precise locations of the warm absorber outflows relative to the putative dusty torus are unknown. A dusty torus is expected to exist around the nuclear source in AGN and be responsible for the IR ‘bump’ seen in their SEDs by reprocessing of the nuclear high energy emission. So there is uncertainty as to how much IR radiation is seen by the warm absorber outflows. In addition, Porquet et al. (2007) report that the 2001 EPIC-pn data show no significant constant narrow 6.4 keV Fe Kα line (with an upper limit of
7.4. Modelling with different Spectral Energy Distributions

Fig. 7.5: The different SEDs (A–H) assumed in the modelling of ESO 113-G010 warm absorber as described in Sects. 7.3 and 7.4, which were used in the ionisation balance calculations. The IR and optical data points (Sect. 7.4.2) are shown as circles and the UV data (Sect. 7.4.3) as squares. The data points in red are corrected only for Galactic extinction as described in Sect. 7.4.1 (panels A and B), whereas the blue data points (in panels C, D, E and F) are also corrected for nuclear obscuration in the AGN as described in Sects. 7.2.1 and 7.2.2. The SEDs in panels C and D have been corrected for nuclear obscuration by using the Balmer decrement and the ones in panels E and F have been corrected for nuclear obscuration by using the continuum reddening. Caption continued on the next page.
7.4. Modelling with different Spectral Energy Distributions

Fig. 7.5: Caption continued from the previous page: In panels C and D, the SEDs with some parts shown in grey and no data points correspond to nuclear obscuration correction with an intrinsic $E(B-V) = 0.64$ (named SEDs C1 and D1) and the ones with blue data points superimposed on the curve correspond to nuclear obscuration correction with an intrinsic $E(B-V) = 0.73$ (named SEDs C2 and D2). The radio point (Sect. 7.4.2) is not displayed in this figure owing to its low flux. The EPIC-pn X-ray data corrected for Galactic absorption are shown as small green circles. The black diamonds correspond to flux at 20 keV extrapolated from the EPIC-pn spectrum, and the extrapolations to the higher energy parts of the SEDs (described in Sect. 7.4.3) are shown as dotted lines. SED G is the SED of Mrk 509 introduced in Sect. 7.3 and used as a ‘standard’ representation for a Seyfert AGN. SEDs on the right-hand side (B, D, F, H) are the same as their adjacent SEDs on the left (A, C, E, G) but without the IR bump and are used in modelling cases where the warm absorber does not receive IR radiation from the dusty torus.

EW < 32 eV), hence suggesting lack of any dominant Compton reflection emission from distant cold matter such as the dusty torus. Thus, to investigate the effect of emission from the dusty torus in the ionisation balance calculations, I consider the same SEDs as described above but without the IR bump (SEDs B, D, F, H in Fig. 7.5) to represent cases in which the outflow does not see emission from the dusty torus.

The above-mentioned SEDs were adopted in my calculations of the ionisation balance and thermal stability curves, as described in Sect. 7.4.5. Note that adopting different SEDs does not affect the goodness of the RGS fits since the columns of the relevant ions detected by the RGS are not significantly different for different SEDs. The parameter which changes significantly as a result of using different SEDs is the ionisation parameter $\xi$, which is given in Fig. 7.6 for each case and plays a significant role in determining the structure of the warm absorber as shown by the thermal stability curves.

7.4.5 Thermal stability curves for the warm absorber

The ionisation balance required for the photoionisation modelling is determined by the SED. The structure of the warm absorber for each SED case in Fig. 7.5 is investigated here. To examine the stability of each warm absorber phase and the possibility of the two phases co-existing in pressure equilibrium, the pressure form of the ionisation parameter, $\Xi$ (see Sect. 3.3), needs to be used. For each SED,
the corresponding thermal stability curve, shown in Fig. 7.6 was produced using the output of the Cloudy runs (described in Sect. 7.3). The best-fit ionisation parameters of phase 1 and phase 2 and their errors are marked on the stability curves. In order for the two phases to co-exist in pressure equilibrium, they must have overlapping values of $\Xi$. These results are discussed in Sect. 7.5.2.

7.5 Discussion

7.5.1 Nuclear obscuration or an intrinsically large Balmer decrement?

Here I discuss several possibilities for the discrepancy between the large Balmer decrement in ESO 113-G010 and the fact that the X-ray spectrum is not intrinsically absorbed by cold neutral gas. From my analysis of the EPIC-pn spectrum, the upper-limit to the neutral gas column density $N_\text{H}$ in ESO 113-G010 (8.9 x 10^{19} cm^{-2}) is much lower than that generally found for a typical Seyfert 1.8 galaxy (4–6 x 10^{21} cm^{-2}, Porquet et al. 2007), in which the BLR is expected to be reddened. Porquet et al. (2007) briefly mentioned possible explanations for such a discrepancy (explanations 1, 2 and 4 which I expand on below), but did not go into details. In this work, with the benefit of my simultaneous optical/UV (OM) and X-ray (RGS, EPIC-pn) analysis of the XMM-Newton data and also analysis of the archival optical spectrum of ESO 113-G010, I can discuss the likelihood of each explanation and suggest which is the most viable solution.

(1) Non-simultaneous optical and X-ray/UV observations

The optical spectrum in which ESO 113-G010 shows the large Balmer decrement was taken in 1996, whereas the XMM-Newton observations were made in 2001 and 2005. The nearest X-ray data to the time of the optical observation were obtained in 1995 by ROSAT. So one can compare the X-ray flux in 2001 and 2005 with the flux in 1995 to check the possibility of variability. As given in Pietsch et al. (1998), the soft X-ray (0.1–2.4 keV) energy flux from the 1995 ROSAT observation is 8.5 x 10^{-12} erg s^{-1} cm^{-2}. I calculate the soft X-ray flux in the same band to be 3.7 x 10^{-12} erg s^{-1} cm^{-2} in 2001 and 5.8 x 10^{-12} erg s^{-1} cm^{-2} in 2005 from the XMM-Newton observations. This flux change over the years is too small to be attributed to occultation by the column of gas inferred from the Balmer decrement in Sect. 7.2.3 $N_\text{H} = (3.5–5.0) \times 10^{21} \text{ cm}^{-2}$. Assuming such a column density of cold
Fig. 7.6: Thermal stability curves (A–H) calculated for the corresponding SEDs of Fig. 7.5. In panels C and D, the curves in blue correspond to SEDs C1 and D1 and those in black to SEDs C2 and D2. The positions of the best-fit warm absorber phases (phases 1 and 2), along with their errors (95.4% confidence level for one interesting parameter) are indicated as thick magenta strips on the curves. Phase 1 is the one with higher $T$. The best-fit ionisation parameters of phases 1 and 2 (i.e. $\xi_1$ and $\xi_2$) in units of erg cm s$^{-1}$ are given for each corresponding stability curve. The dotted lines are plotted for display purposes to show the range of $\Xi$ for one of the phases on each curve. The regions overlapping in $\Xi$ on each stability curve are in pressure equilibrium.
gas was present during the optical observation and the unabsorbed soft X-ray flux was at the same level as in 2001 or 2005 (when it is known there was no intrinsic neutral absorption) would imply an obscured soft X-ray flux smaller by a factor of 3.1–4.1, whereas in 1995 the X-ray flux was actually larger by a factor of 1.5–2.3.

More importantly, during the 2005 XMM-Newton observation, when simultaneous UV (4 UV filters of OM) and X-ray observations are available, the optical/UV continuum, which is supposed to represent thermal emission from the accretion disc, appears to be intrinsically reddened as described in Sect. 7.2.2. So the non-simultaneity of the optical spectroscopy and X-ray observations is unlikely to be the cause of discrepancy between the reddening and X-ray neutral absorption.

(2) Partially covering neutral gas clouds

The clouds of neutral gas and dust that obscure the NLR and BLR may only partially cover the nuclear source, such that they are not in our line of sight to the X-ray emitting region. This way optical emission from the NLR and BLR is reddened but the X-rays remain unabsorbed. This scenario is however an unlikely possibility as it requires an ad hoc geometry of the absorbing regions. Furthermore, since the slope of the optical/UV continuum shows that intrinsic UV emission from the accretion disc has been reddened, the intrinsic X-ray emission originating from the corona in close vicinity of the disc must also have passed through the same material as the UV emission. Therefore, partially covering neutral gas clouds in the host galaxy of the AGN are not a feasible solution.

(3) Intrinsically large Balmer decrements

One possible explanation is that Balmer decrements are intrinsically large for the BLR or even the NLR. The physical conditions in the BLR are to some extent uncertain and higher density clouds within the BLR can cause collisional and radiative effects which can raise the value of the intrinsic Balmer decrement, e.g. from 3 to 10 (Kwan and Krolik 1981).

Barcons et al. (2003a) have analysed the optical (WHT) and X-ray (XMM-Newton EPIC-pn) spectra of the Seyfert 1.8/1.9 galaxy H1320+551. They find that the Balmer decrement $H\alpha/H\beta$ is about 6 for the NLR and about 27 or more for the BLR. Despite such large Balmer decrements, the X-ray spectrum is not intrinsically absorbed. They find a 3$\sigma$ upper limit of $1.4 \times 10^{20}$ cm$^{-2}$ to the obscuring column.
density, which they report is about 7 and 70 times smaller than the minimum predicted from the NLR and BLR Balmer decrements respectively. Barcons et al. (2003a) also rule out the existence of an ionised absorber in H1320+551 from their X-ray spectral fits. They suggest the large Balmer decrement of the BLR is an intrinsic property and not caused by internal reddening, and so H1320+551 is not consistent with being an obscured Type-1 Seyfert AGN.

However, in ESO 113-G010, the UV continuum provides an estimate of the reddening independent from that inferred from the Balmer decrement. As shown in Sect. 7.2.2, the amount of reddening derived from the continuum study, $E(B-V) = 0.39$, is less than that inferred from the Balmer decrement, $E(B-V) = 0.64 - 0.73$. This may indicate that the Balmer decrement over-estimates the amount of reddening, as the intrinsic Hα/Hβ is larger than the theoretical values 3.1–3.5.

From Eq. 7.2, the intrinsic Hα/Hβ needs to be about 4.8 in order to imply $E(B-V) = 0.39$, while the value observed is $\sim 8$. One reason against the large reddening obtained from the Balmer decrement is that the bolometric luminosity calculated from the de-reddened SEDs (SEDs C1 and C2 in Fig. 7.5) is high for a Seyfert galaxy: $2.8-5.8 \times 10^{46}$ erg s$^{-1}$; on the other hand, the bolometric luminosity of the SED de-reddened using the continuum (SED E in Fig. 7.5) is $4.7 \times 10^{45}$ erg s$^{-1}$. This is very similar to the bolometric luminosity of Mrk 509, calculated from SED G: $4.6 \times 10^{45}$ erg s$^{-1}$. Nonetheless, even if to some degree the large Balmer decrement is intrinsic, the slope of the optical/UV continuum indicates there must be intrinsic reddening taking place in our line of sight to ESO 113-G010.

(4) Dusty warm absorber

The most viable explanation for the discrepancy between the reddening and X-ray absorption in ESO 113-G010 is that the X-ray warm absorber contains dust. The dust causes the observed optical/UV reddening of the continuum and the large Balmer decrement, whilst the X-rays remain photoelectrically unabsorbed since the gas in the warm absorber is ionised (predominantly owing to the ionisation of carbon and oxygen), and the X-ray opacity of dust is lower than that of cold neutral gas. This means unusually large dust-to-gas ratio clouds in the ISM of the host galaxy are not needed to explain the discrepancy between reddening and X-ray absorption. Previous studies show that dust particles can survive the dust destruction mechanisms (sublimation and thermal sputtering) under conditions found in some warm
absorbers. For example, Reynolds et al. (1997b) suggest the existence of a dusty warm absorber in the Seyfert-1 galaxy MCG $-$6-30-15 to account for the discrepancy between the reddening and lack of X-ray absorption by neutral gas, and discuss the survival of dust grains under conditions found in a photoionised warm absorber. In the following I check if dust can survive in the warm absorber of ESO 113-G010.

As shown in Barvainis (1987), the sublimation radius (the minimum distance from the central source at which particular grains can exist) for graphite grains is given by

$$R_{\text{sub}} = 1.3 L_{\text{uv},46}^{0.5} T_{1500}^{-2.8} \text{ pc},$$

(7.3)

where $L_{\text{uv},46}$ is the UV luminosity of the central source in units of $10^{46}$ erg s$^{-1}$, and $T_{1500}$ is the graphite grain sublimation temperature in units of 1500 K. Taking an upper estimate of $10^{46}$ erg s$^{-1}$ for the UV luminosity of ESO 113-G010 (consistent with my SEDs), one obtains $R_{\text{sub}} \sim 1.3$ pc. So as long as the dust resides in a warm absorber phase which is further than 1.3 pc from the source, it is not destroyed by sublimation.

Another mechanism that can destroy dust grains is sputtering, in which atoms or molecules are knocked off the surface of the dust grain due to collisions with hot ions. As given in Burke and Silk (1974), the threshold for sputtering graphite grains corresponds to a gas temperature of about $4 \times 10^5$ K. Burke and Silk (1974) have shown that above the sputtering threshold, the grain lifetime against destruction by sputtering is

$$t_{\text{sput}} = 6.25 \times 10^{11} (Y n T_{\text{4}}^{0.5})^{-1} \text{ s},$$

(7.4)

where $Y$ is the sputtering yield at $T_4$, the incident particle energy in units of $10^4$ K, and $n$ is the incident particle density. Phase 2 of the warm absorber in ESO 113-G010 has a maximum temperature of $2.6 \times 10^5$ K corresponding to SED C1 (see Fig. 7.6). This temperature is below the sputtering threshold and thus graphite dust grains in phase 2 should not be destroyed by the sputtering mechanism. On the other hand, phase 1, which is hotter than phase 2, has a minimum temperature of $9.3 \times 10^5$ K (corresponding to SED G) and a maximum temperature of $2.7 \times 10^6$ K (corresponding to SED A). So the temperature of phase 1 is higher than the sputtering threshold for all SED cases. Substituting $n$ from the expression of the ionisation parameter ($\xi = L/nr^2$) into that of $t_{\text{sput}}$ (Eq. 7.4), one finds that
7.5. Discussion

for phase 1 (with the parameter values given in Table 7.3), $t_{\text{sput}} \sim 22.8r^2$ yr, where $r$ is the distance of the gas from the central source in pc. Furthermore, one can roughly estimate phase 1 flow timescale, $t_{\text{flow}} \sim r/v$, where $v$ is the velocity of phase 1 (i.e. $1100 \text{ km s}^{-1}$); so $t_{\text{flow}} \sim 890r$ yr, where the distance $r$ is in pc. The dust grains are destroyed by sputtering if $t_{\text{sput}} < t_{\text{flow}}$; therefore, if $r < 39$ pc, then the dust grains in phase 1 cannot survive the sputtering. Assuming a constant velocity outflow, an upper limit for the distance $r$ can be estimated by using $N_H = n r f$ to substitute into $\xi = L/nr^2$ and eliminate $n$, where I take the volume filling factor $f = 1$. For phase 1, one obtains $r < 52$ pc, so the dust grains can only survive in phase 1 if $39 < r < 52$ pc. However, phase 2 (with $r < 1.3$ kpc applying the same calculations as above), which is the lower-ionised phase of the warm absorber with a temperature below the sputtering threshold, is more likely to host dust grains than phase 1.

7.5.2 The structure of the warm absorber

From modelling of the RGS spectrum, I found that the warm absorber in ESO 113-G010 consists of at least two phases of ionisation. As shown in Table 7.3, the higher-ionised phase 1 has a larger column density than the lower-ionised phase 2, and also has larger outflow and RMS velocities. The thermal stability curves of Fig. 7.6 show that depending on which ionising SED is selected, quite different stability curves are obtained. The SED also dictates whether the absorber phases lie on the stable or unstable part of the curves. Only in case C, in which the optical/UV continuum is de-reddened using the Balmer decrement and the warm absorber does receive IR radiation from the dusty torus of the AGN, the two phases have overlapping values of $\Xi$ and hence can be in pressure equilibrium. However, for all other cases, the two phases do not overlap in $\Xi$, so they are not in pressure equilibrium. Since also their velocities are different, I conclude that the two phases are likely to be separated and out of pressure equilibrium.

The exact location of the warm absorber relative to the dusty torus is unknown, so it is not clear whether or not the warm absorber sees IR radiation from the torus. As mentioned in Sect. 7.4.4, from analysis of the Fe Kα line, Porquet et al. (2007) report lack of Compton reflection from distant cold regions such as the dusty torus. However, lack of Compton reflection from cold matter does not imply absence of a dusty torus, because the BLR is likely to be obscured by the torus given the lack of
broad optical emission lines in this object; also it does not imply the warm absorber
is not receiving IR emission from the torus because the warm absorber phases (most
likely evaporated off the torus itself) are likely to be further away from the torus
(see the \( r \) values derived in the previous section), so they may see IR radiation from
the outer parts of the torus. As inferred from Fig. 7.6 apart from cases C and D,
presence or not of IR radiation from the dusty torus does not affect whether or not
the two phases are in pressure equilibrium anyway.

As discussed earlier, dust can survive in the lower-ionised phase (phase 2) of the
warm absorber, which can account for the discrepancy between the large optical/UV
reddening and the low amount of X-ray neutral absorption in ESO 113-G010. Since
the NLR is reddened as inferred from the Balmer decrement, then the dust in phase
2 of the warm absorber cannot be closer to the nucleus than the NLR. So phase
2 of the warm absorber must lie somewhere between the NLR and the maximum
distance of 1.3 kpc at which the absorber can be kept photoionised. Spatially
resolved NLRs (see Sect. 2.2.2) in nearby Seyferts show diameters of order 10^2–
10^3 pc (e.g. Osterbrock and Ferland 2006). The range of possible distances from
the nucleus for the dusty warm absorber (phase 2) overlaps the range which the
NLR is likely to occupy, so the two regions could be co-spatial. On the other hand,
the higher-ionised phase 1, which is not co-spatial with phase 2 on the grounds of
thermal stability analysis and different outflow velocities, has \( r < 52 \), which places
it interior to phase 2 and the NLR.
Chapter 8

Conclusions and implications

This thesis describes the research I have carried out on three AGN of similar classification (Seyfert 1 galaxies), but with each showing distinctive characteristics in some of the different facets of the AGN make-up: the large and fast variability of the Seyfert 1.5 NGC 3516, the shallower and spectrally correlated modulation of the QSO/Seyfert 1 hybrid Mrk 509, and the dusty warm absorber in the Seyfert 1.8 ESO 113-G010. I have used the results obtained on these three objects to draw conclusions on their inner physical structures, to suggest implications for AGN in general and the relevance of this to feedback and AGN-host galaxy evolution.

8.1 Variability and warm absorption in NGC 3516

I have studied the warm absorber in NGC 3516 by analysing in detail simultaneous EPIC-pn and RGS high resolution spectra from four observations made in October 2006 by \textit{XMM-Newton}. The warm absorber consists of three phases of ionisation: phase A (log \( \xi \sim 0.9 \)), phase B (log \( \xi \sim 2.4 \)) and phase C (log \( \xi \sim 3.0 \)) in increasing order of ionisation. Phase A has a hydrogen column density of \( \sim 0.4 \times 10^{22} \text{ cm}^{-2} \), which is smaller than those of the other two phases (\( \sim 1.2 \times 10^{22} \text{ cm}^{-2} \)). There is evidence that the lower-ionisation phase A is outflowing at \( \sim 100 \text{ km s}^{-1} \), whereas the two higher-ionisation phases are outflowing faster at around 1000 to 1500 km s\(^{-1}\). Furthermore, the three warm absorber phases in NGC 3516 are found not to be in pressure equilibrium with each other.

Phase B covers about 60% of the source continuum. I investigated whether variation in the covering fraction of phase B could account for the observed flux and spectral variability in Obs. 3 (as claimed by Turner et al. 2008). I found that (1)
the covering fraction does not show significant variation between observations; (2) even if the covering fraction is altered significantly, this does not properly account for the observed variability in the EPIC-pn and especially RGS spectra. This makes a clumpy disc-wind scenario a rather unfeasible explanation.

Similarly to Netzer et al. (2002), I conclude that the variability in the 2006 observations presented here (albeit much smaller than in previous observations of NGC 3516) is better understood as the consequence of changes in the source continuum emission than in the warm absorber. My results suggest that the X-ray variability of NGC 3516 (and by inference, possibly that of other AGN where a similar behaviour has been observed) cannot be reduced to occultation and absorption effects, such as proposed by Turner et al. (2008) (see also review by Turner and Miller 2009, and references therein); rather, the variability is likely to arise in a scenario where intrinsic changes of the continuum and ionisation state are also important. In this context, a careful analysis of the soft X-ray spectrum at high resolution, in combination with spectral data at higher energies, can provide essential constraints and clues to the source’s physical behaviour.

8.2 The nature and origin of the soft X-ray excess in Mrk 509

In order to study the intrinsic optical/UV and X-ray continuum of the Seyfert-1/QSO hybrid Mrk 509 (using XMM-Newton OM and EPIC-pn, Swift UVOT and XRT, HST/COS and FUSE), I have taken into account various processes occurring in our line of sight towards the central source, such as Galactic reddening and absorption, host galaxy emission, BLR and NLR emissions and the AGN multiphase warm absorption. The optical/UV continuum of Mrk 509 is found to be consistent with thermal emission from a geometrically thin, optically thick accretion disc with a maximum temperature of about 2 eV. The X-ray continuum can be represented by two distinct components: a power-law with photon index $\Gamma \sim 1.9$ and a soft X-ray excess below 2 keV. I investigated the variability of the optical/UV and X-ray continuum of Mrk 509 over the 100 days of a monitoring campaign with a resolution of a few days. The variability of the soft X-ray excess is found to be very similar in profile to that of the optical/UV emission from the disc. The flux variability of the higher energy X-ray power-law component (albeit smaller), on the
other hand, is uncorrelated with the variability of the soft X-ray excess and that of
the disc emission over the probed timescales. There is however correlation between
the power-law photon index and the disc blackbody flux.

I conclude that in Mrk 509 the origin of the soft X-ray excess and its variability
can be accounted for by Comptonisation of the disc photons in a warm (about
0.2 keV), optically thick ($\tau \sim 17$) corona surrounding the inner disc. The X-ray
power-law is likely to originate from Comptonisation in a separate optically-thin
hot corona, in the form of an atmosphere surrounding the disc. Explaining the
soft X-ray excess using warm Comptonisation has previously been suggested for the
Seyfert-1 NGC 5548 and the NLS1s: RE J1034+396 and RX J0136.9-3510. This
interpretation is analogous to the inner-disc warm-corona model which explains the
existence of the high-energy tail observed in some Black Hole Binaries spectra in
the Very High State. Mrk 509 is the highest mass black hole system known to
display such variability and thus to call for the suggested origin of the soft excess. I
conclude that variability studies based on multi-wavelength monitoring campaigns,
such as the one reported in this work, are a unique and invaluable tool for detailed
investigations of the processes leading to the formation of AGN broad-band spectra.

8.3 Obscuration and warm absorption in ESO 113-G010

The first-ever study of the X-ray warm absorber and nuclear obscuration in the
Seyfert 1.8 ESO 113-G010 was presented as part of this thesis. I found that the warm
absorber detected by the XMM-Newton RGS consists of two phases of ionisation,
with $\log \xi \approx 3.2$ and 2.3 respectively. The higher-ionised component (phase 1),
with $N_H \approx 1.6 \times 10^{22}$ cm$^{-2}$, is outflowing with $v \approx -1100$ km s$^{-1}$; the lower-ionised
component (phase 2), with $N_H \approx 0.5 \times 10^{22}$ cm$^{-2}$, moves out with $v \approx -700$ km s$^{-1}$.

ESO 113-G010 displays a large Balmer decrement ($H_{\alpha}/H_{\beta} \sim 8$) relative to
the theoretical predictions for the NLR and BLR, implying a significant amount
of reddening with $E(B-V) = 0.64 - 0.73$ and a large column of cold gas, with
$N_H = (3.5 - 5.0) \times 10^{21}$ cm$^{-2}$, in the host galaxy of the AGN. However, the X-ray
spectrum is not absorbed by such a column of gas; from the XMM-Newton data I
find an upper limit of $8.9 \times 10^{19}$ cm$^{-2}$ for the neutral hydrogen equivalent column
density $N_H$. Alternative explanations for the discrepancy between the large Balmer
decrement and lack of X-ray absorption are discussed in this thesis. I find that
partially covering gas clouds or an intrinsically large Balmer decrement are not feasible solutions since the shape of the optical/UV continuum flux (supposed to be thermal emission from the accretion disc) also indicates reddening. I suggest that dust embedded in a warm absorber is a viable explanation for the discrepancy, without requiring unusually large dust-to-gas ratio clouds in the ISM of the host galaxy. Graphite dust grains can survive the sublimation and sputtering processes in the lower-ionised phase of the warm absorber, and thus can cause the observed optical/UV reddening, whereas the X-rays remain unabsorbed due to lack of a substantial column of neutral gas in the ionised absorber. The dusty phase of the warm absorber in ESO 113-G010 is likely to be co-spatial with the NLR.

I have then explored the uncertainties in the construction of the SED and ultimately on the ionisation balance calculations required for photoionisation modelling of ESO 113-G010 owing to its nuclear obscuration and the effects these have on the results of my warm absorber analysis. The only parameter of the warm absorber outflows which significantly changes as a consequence of using different SEDs is the ionisation parameter. Furthermore, different SEDs result in different thermal stability curves, which determine whether or not the two phases of the warm absorber are in pressure equilibrium. I find that only for the case where the SED is corrected for reddening in the host galaxy using the Balmer decrement, and the warm absorber does receive IR radiation from the dusty torus expected to surround the AGN, the two phases of ionisation can co-exist in pressure equilibrium on the thermal stability curve, whereas for other SEDs the two phases are distinct and not in pressure equilibrium. I conclude that the two phases of the warm absorber in ESO 113-G010 are most likely to be spatially separated and not in pressure equilibrium with each other. This work demonstrates the importance of establishing the intrinsic broad-band SED in order to interpret correctly the structure of the warm absorber in AGN.

The obscuring molecular torus in the AGN unification scheme is expected to be a reservoir of dusty material. In fact, the large IR bump in Type-2 AGN spectra is modelled well with thermal emission from dusty material heated by the continuum emission (e.g. Barvainis 1987). The dusty torus model (Pier and Krolik 1993) is also supported by reverberation studies in the optical and near-IR bands, which have found a clear time-delayed behaviour in the K-band with respect to the op-
tical/UV continuum, suggesting that the bulk of the K-band emission originates from thermal emission of dust grains in an optically thick torus (see e.g. Glass 2004; Suganuma et al. 2006). For example, Suganuma et al. (2006) find K-band lag-times ranging from 10 to 80 days with respect to the V-band for four Seyfert-1 AGN, which is interpreted as representing the light travel-time from the central source to the inner-edge of the dusty torus. The observed evidence of dust in warm absorbers, such as the one reported in ESO 113-G010 in this thesis (as well as in MCG −6-30-15, Reynolds et al. 1997b), suggests a radiatively-driven dusty wind outflowing from the inner-edge of the dusty torus. Because of its large cross-section, dust is subjected to a large radiation force which is then delivered to the ionised gas through the efficient charge coupling of the two components; in fact radiation pressure acceleration imparted to dust can be orders of magnitude larger than that imparted to gas (see e.g. review of Netzer 2008). Therefore, understanding the role of dust in ionised outflows is crucial in defining the contribution of outflows to AGN feedback (see Sect. 9.2). Furthermore, the NLR in AGN is widely known to contain dust (e.g. Netzer and Laor 1993), thus it is likely that the radiatively driven outflows transport dust from the dusty torus to the NLR, and eventually into the host galaxy.
Chapter 9

Future work

Understanding the physics and demographics of feedback via ionised outflows is an important part of AGN science. In 2014 the first ever cryogenic X-ray spectrometer will fly on-board Astro-$H$, enabling high resolution observations in the Fe K$\alpha$ energy band as well as in the soft X-rays. This will provide unprecedented opportunities to study the physical properties of the higher-velocity and higher-ionised outflows, which are too weak to be detected in the soft X-rays and cannot be resolved by the existing hard X-ray spectrometers. High-resolution spectroscopy of AGN ionised outflows will consequently be a significant part of X-ray studies of AGN from 2014 onwards, and it is here that I believe the work presented in this thesis can develop into further research. Studies of outflows have so far outlined the qualitative characteristics of these phenomena, and produced quantitative results in a few cases, but we are still missing the in-depth understanding. Along with Astro-$H$, systematic, strategically targeted studies with XMM-$Newton$ and Chandra will give a higher definition picture of the AGN power sources and their impact on the environment around them. As a natural progression from what has been presented in this thesis, my approach to studying feedback processes in AGN would target the following specific goals.

9.1 Demographic survey of ionised absorber outflows

A comprehensive and homogeneous demographic survey of ionised absorbers and their physical parameters in the nearby Universe needs to be constructed. The initial strategy would be to produce a comprehensive survey of local, un-obscured AGN outflow properties and demographics, building on the work of Bhustin et al.
9.2 Dust and cool gas in the ionised absorber outflows

(2003), which drew on a limited amount of high resolution spectra available only a few years into the XMM-Newton and Chandra missions. There are now several times more data available in archives, and a careful treatment of selection effects and a uniform approach to the analysis are needed.

Establishing the distances to the ionised absorbers, or at least stringent limits (see Sect. 3.6 and e.g. Kaastra, Detmers, Mehdipour et al. 2012) is indispensable in order to discriminate between the different outflow mechanisms, and to measure the mass outflow rates and kinetic luminosities, which are core parameters in assessing the impact that outflows have on their surroundings.

9.2 Dust and cool gas in the ionised absorber outflows

The interaction of ionised gas with dust and cool material at the heart of AGN also needs investigating. With the recent Herschel discovery that a molecular outflow accompanies the ionised wind in Mrk 231 (Fischer et al. 2010), it is clear that the interaction between ionised winds and cold, dusty material is fundamental to understanding the process by which AGN feedback quenches star formation. Dust likely acts as a force multiplier in radiatively driven outflows, and probably also acts as a shield for the cool, molecular phase of the gas. My case-study of ESO 113-G010 could be expanded to a sample of nearby galaxies which show dust obscuration in the optical and UV as well as signs of ionised outflows with little or no cold absorption in soft X-rays.

The main issues are how and where dust can co-exist with ionised gas, and to what extent this is controlled by the highest ionisation phases of the outflow; how the presence of dust changes the character of the outflow, and especially how it affects its velocity (given the large dust cross-section for radiative driving), and how the dynamics of the different phases compare and relate to each other. Answers to these questions can emerge from a systematic and uniform survey of outflow signatures which can be carried out with high resolution soft X-ray spectra already obtained by XMM-Newton and Chandra as well as with upcoming Astro-H data covering both the soft and hard X-ray bands.

There is the prospect of more in-depth high-resolution X-ray spectroscopy of dust embedded in AGN ionised outflows by using future X-ray missions with higher throughput and spectral resolution than the current ones. In much the same way
ions are identified by their absorption/emission lines, spectral modulations near photoelectric edges (known as X-ray absorption fine-structures) would provide signatures of dust particles, from which their quantity and chemical composition can be studied (see [Lee et al. 2009]). In the near future, the high-resolution soft X-ray microcalorimeter spectrometer (SXS) onboard the Astro-H mission could make it possible to investigate the properties of dust in AGN ionised outflows (see [Lee 2010]).

9.3 Linking inflows and outflows in AGN

The physical connection between the accretion-powered high energy emission and the outflowing, ionised gas in AGN has still to be established. Rudimentary relationships between outflows and accretion are known (e.g. that the fastest outflows occur only in sources emitting at high Eddington ratios), but deeper understanding has been hampered by the disparate nature of data on ionised absorber parameters and the lack of progress in de-convolving the various contributions to the AGN emission spectra. To investigate the connection between the accretion process and the ionised outflows, the detailed and homogeneous characterisation of the outflows outlined in Sect. 9.1 could be combined with precise measurements and decomposition of the accretion radiation spectrum in the brightest nearby AGN. The outflows exhibit a wide range of physical properties (velocities, column densities, ionisation parameters, etc.). As they are ultimately driven by the accretion process, their properties are related to the physical conditions and/or radiation spectra of the accretion disc and associated components (the Compton-scattering X-ray corona, and the cooler scattering region proposed to be responsible for the soft X-ray excess). Unraveling this scenario involves exploring and understanding complex atomic processes coupled with hydrodynamics: this is science that bridges the micro-scale (in this context, the AGN), the meso-scale (the outflow) to the macro-scale (the AGN environment and the host galaxy).

In practice this could be tackled with a systematic study of the optical/UV/X-ray time variability of a sample of nearby Seyfert AGN which have been targets of XMM-Newton with multiple long observations by the EPIC/RGS for the X-ray and the OM for the optical/UV, so that their different components of intrinsic emission could be de-convolved and their origin investigated. As demonstrated for Mrk 509 in this thesis and in [Mehdipour et al. 2011], correlating the variability in different
9.3. Linking inflows and outflows in AGN

energy ranges provides the crucial discriminant for the origin of the soft X-ray emission, which can be separated, identified and characterised in broadband spectral modelling. These observational results would constrain the input parameters for the radiative transfer calculations that determine the energy distribution through the AGN system and can ultimately clarify how the radiation generated by accretion drives the outflows.

Fundamental aspects of AGN science will be clarified and better understood through the research outlined above. Apart from influencing their immediate surroundings in the core of AGN, inflows and outflows have far-reaching consequences on a much larger scale. The balance between accretion and outflows impacts the growth of SMBHs, as well as the growth and evolution of their host galaxies through feedback processes, the enrichment of the surrounding IGM and the cooling flows at the cores of clusters of galaxies. Furthermore, by expanding the study of inflows/ionised-outflows to black hole systems of various scales and accretion rates, one can investigate their fundamental similarities and differences. Which physical parameters regulate inflows and outflows, how is the energy budget distributed between inflows, outflows and radiation in various black hole systems (AGN to BHBs), and what are the implications on their environment and beyond: these are fundamental and fascinating questions still much to be explored in high-energy astrophysics.
List of common abbreviations

Acronyms

AGN  active galactic nuclei
ASCA  Advanced Satellite for Cosmology & Astrophysics
BHB  black hole binary
BLR  broad-line region
BLRG  broad-line radio galaxy
CCD  charge-coupled device
COS  Cosmic Origin Spectrograph
d.o.f.  degrees of freedom
ENLR  extended narrow-line region
EPIC  European Photon Imaging Camera
ESA  European Space Agency
EUVE  Extreme Ultraviolet Explorer
EW  equivalent width
EXOSAT  European X-ray Observatory Satellite
FR  Fanaroff and Riley
FUSE  Far Ultraviolet Spectroscopic Explorer
FWHM  full-width-half-maximum
GTI  good time interval
HEAO  High Energy Astronomy Observatory
HETGS  High Energy Transmission Grating Spectrometer
HEW  half-energy-width
HST  Hubble Space Telescope
IGM  intergalactic medium
INTEGRAL  International Gamma-Ray Astrophysics Laboratory
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>ISF</td>
<td>inverse sensitivity function</td>
</tr>
<tr>
<td>ISM</td>
<td>interstellar medium</td>
</tr>
<tr>
<td>IUE</td>
<td>International Ultraviolet Explorer</td>
</tr>
<tr>
<td>LETGS</td>
<td>Low Energy Transmission Grating Spectrometer</td>
</tr>
<tr>
<td>Mrk</td>
<td>Markarian</td>
</tr>
<tr>
<td>NED</td>
<td>NASA/IPAC Extragalactic Database</td>
</tr>
<tr>
<td>NLR</td>
<td>narrow-line region</td>
</tr>
<tr>
<td>NLRG</td>
<td>narrow-line radio galaxy</td>
</tr>
<tr>
<td>NLSy1</td>
<td>narrow-line Seyfert-1 galaxy</td>
</tr>
<tr>
<td>ODF</td>
<td>Observation Data Files</td>
</tr>
<tr>
<td>OM</td>
<td>Optical Monitor</td>
</tr>
<tr>
<td>OVV</td>
<td>Optically Violently Variable quasar</td>
</tr>
<tr>
<td>PG</td>
<td>Palomar-Green</td>
</tr>
<tr>
<td>PIE</td>
<td>photoionisation equilibrium</td>
</tr>
<tr>
<td>PSF</td>
<td>Point Spread Function</td>
</tr>
<tr>
<td>QSO</td>
<td>quasi-stellar object</td>
</tr>
<tr>
<td>RGA</td>
<td>Reflection Grating Array</td>
</tr>
<tr>
<td>RGS</td>
<td>Reflection Grating Spectrometer</td>
</tr>
<tr>
<td>ROSAT</td>
<td>Roentgen Satellite</td>
</tr>
<tr>
<td>RQQ</td>
<td>radio-quiet quasar</td>
</tr>
<tr>
<td>RRC</td>
<td>radiative recombination continua</td>
</tr>
<tr>
<td>RXTE</td>
<td>Rossi X-ray Timing Explorer</td>
</tr>
<tr>
<td>SAS</td>
<td>Small Astronomical Satellite; Science Analysis Software</td>
</tr>
<tr>
<td>SDSS</td>
<td>Sloan Digital Sky Survey</td>
</tr>
<tr>
<td>SED</td>
<td>spectral energy distribution</td>
</tr>
<tr>
<td>SMBH</td>
<td>supermassive black hole</td>
</tr>
<tr>
<td>ULIRG</td>
<td>ultra-luminous infrared galaxy</td>
</tr>
<tr>
<td>UTA</td>
<td>Unresolved Transition Array</td>
</tr>
<tr>
<td>UVOT</td>
<td>UV/Optical Telescope</td>
</tr>
<tr>
<td>WFPC</td>
<td>Wide Field and Planetary Camera</td>
</tr>
<tr>
<td>WHT</td>
<td>William Herschel Telescope</td>
</tr>
<tr>
<td>XRT</td>
<td>X-ray Telescope</td>
</tr>
</tbody>
</table>
Symbols

c speed of light

$C_f$ covering fraction

$C_g$ global covering fraction

$F_\nu$ flux density

$G$ gravitational constant

$h$ Planck constant

$k_B$ Boltzmann constant

$L$ luminosity

$L_{\text{bol}}$ bolometric luminosity

$L_k$ kinetic luminosity

$M$ black hole mass

$M_{\odot}$ mass of the Sun

$\dot{M}$ mass accretion rate

$n_e$ electron density

$n_i$ density of ions in ionisation state $i$

$N_H$ hydrogen column density

$r$ distance from a central black hole

$R_g$ gravitational radius

$R_S$ Schwarzschild radius

$t_{\text{rec}}$ recombination timescale

$T_e$ electron temperature

$v$ flow velocity

$\alpha_{i+1}$ recombination rate coefficient from state $i + 1$ to $i$

$\beta_i$ photoionisation rate from state $i$ to $i + 1$

$\gamma$ Lorentz factor

$\Gamma$ power-law photon index

$\Delta t$ lag time

$\nu$ frequency

$\xi$ ionisation parameter

$\Xi$ pressure form of the ionisation parameter

$\sigma$ Stefan-Boltzmann constant
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
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<tbody>
<tr>
<td>$\sigma_{ph}$</td>
<td>photoionisation cross-section</td>
</tr>
<tr>
<td>$\sigma_T$</td>
<td>Thomson cross-section</td>
</tr>
<tr>
<td>$\sigma_v$</td>
<td>RMS velocity</td>
</tr>
<tr>
<td>$\tau$</td>
<td>optical depth</td>
</tr>
<tr>
<td>$\chi$</td>
<td>photoionisation threshold energy</td>
</tr>
<tr>
<td>$\chi^2_\nu$</td>
<td>reduced chi-squared (goodness of fit measure)</td>
</tr>
</tbody>
</table>
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Publications

First-authored


Co-authored


