Absorption spectra of Fe L-lines in Seyfert 1 galaxies

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Abstract

Absorption L-lines of iron ions are observed, in absorption, in spectra of Seyfert 1 galaxies by the new generation of X-ray satellites: Chandra (NASA) and XMM-Newton (ESA). Lines associated to Fe\textsuperscript{23+} to Fe\textsuperscript{17+} are well resolved. Whereas, those corresponding to Fe\textsuperscript{16+} to Fe\textsuperscript{6+} are unresolved. Forbidden transitions of the Fe\textsuperscript{16+} to Fe\textsuperscript{6+} ions were previously observed, for the same objects, in the visible and infra-red regions, showing that the plasma had a low density. To interpret X-ray, visible and infra-red data, astrophysical models assume an extended absorbing medium of very low density surrounding an intense X-ray source. We have calculated atomic data (wavelengths, radiative and autoionization rates) for \( n=2 \) to \( n'=3-4 \) transitions and used them to construct refined synthetic spectra of the unresolved part of the L-line spectra.

Key words: X-ray; absorption lines; atomic processes

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1 Introduction

The new generation of X-ray satellites (Chandra and XMM-Newton) produces very detailed spectra, thanks to a high spectral resolution combined to a high sensitivity of the spectrometers on board. For the first time, it is possible to have access to X-ray spectroscopy of extra-solar astrophysical objects: e.g., stellar coronae, Active Galactic Nuclei (AGN), X-ray binaries, etc. In particular, observations of Seyfert galaxies, show numerous lines of highly ionized elements: predominantly in absorption, for Seyfert 1 and only in emission for Seyfert 2 galaxies.

Much atomic data have already been calculated to analyze X-ray spectra of solar corona or laboratory plasmas. The well-known He-like ion diagnostics [1], [2] have been extended from solar to non-solar coronae and also to photoionized plasmas [3], [4]. Besides these K-lines, Fe-L lines have also been observed in X-ray spectra, for Seyfert 1 [5](Fig. 1), [6], [7] and for Seyfert 2 [8] (Fig.2) galaxies. To analyze the unresolved part of the Fe-L spectra (Fe$^{16+}$ to Fe$^{6+}$), atomic data for the transitions from n=2 to n’=3 have been calculated and presented as an abbreviated set, assuming a UTA (unresolved transition array) statistical model [9], i.e. mean wavelengths, statistical spectral widths of transition arrays, etc. The arguments used by the authors to justify statistical treatment is that various processes, such as turbulence, will merge lines into a broad UTA, independent of the spectral resolution of the measuring device. Comparisons of the Seyfert 1 NGC 3783 spectra with different spectral resolutions (see Tables 1), XMM [6] and Chandra [7] (Fig 3), show that the statistical assumption is not justified at least for this object. In Fig. 3, finer detail can be clearly resolved. Indeed, for such a low density
plasma the number of possible absorption transitions is quite limited and as
the absorption changes dramatically over the ionization stages (see Tables 2,
3) the use of a statistical width artificially increases the real width of the lines.
We have therefore re-calculated all the atomic data of [9], extending them to
n’= 4 transitions, giving a particular importance to the numerous possible
autoionization channels.

2 Seyfert Galaxies

Seyfert galaxies, discovered by Seyfert [10], have very compact and bright cen-
ters, the so-called Active Galactic Nuclei (AGN): their bolometric luminosities
(i.e., including all wavelength contributions) \( L_{\text{bol}} \sim 10^{10}-10^{11}L_{\odot} \), \( L_{\odot} \) being the
solar bolometric luminosity. The surrounding stars are relatively faint com-
pared to the central nucleus. These galaxies are relatively close to our galaxy
exhibiting small red-shifts (\( z \equiv \Delta \lambda / \lambda \leq 0.05 \)). Seyfert galaxy optical spectra
show strong emission lines of ionized gas plus a non-stellar continuum. The
energy power from the galactic nucleus is commonly supposed to be due to
some super-massive black hole (\( M_{\text{BH}} \sim 10^6-10^9 M_{\odot} \), (where \( M_{\odot} \) is the solar
mass)) surrounded by an accretion disk (see Fig. 4). This disk is observed in
emission in all wavelengths from X-ray to infra-red.

There are two types of Seyfert galaxies: the Seyfert 1 and the Seyfert 2, dis-
tinguished by their observed visible spectra. The Seyfert 1 show both broad
(Full Width at Half Maximum: FWHM\( \sim 2000—20000 \text{ km s}^{-1} \)) and narrow
(FWHM\( \leq 2000 \text{ km s}^{-1} \)) lines, while Seyfert 2 exhibit only narrow lines. How-
ever, Antonucci & Miller [11], in the NGC 1068 Seyfert 2, detected also broad
lines using polarimetry. This led to the conjecture that Seyfert 1 and Seyfert
2 are the same type of objects but viewed with different angles. That is, for Seyfert 1, the observer views the central continuum source which is the “Broad Line Region” while, in Seyfert 2, the observer views the external part or the “Narrow Line Region”, due to obscuration of the central continuum source by some molecular torus (see Fig. 3). This model is supported by the discovery in the X-ray spectrum of a dilute and high ionization medium called the “Warm Absorber” (discovered by Halpern [13] in MR2251-178), mainly observed in absorption in Seyfert 1, while only seen in emission in Seyfert 2 (e.g., Kinkhabwala et al.[8]).

3 Calculations of atomic parameters

3.1 Method

Wavelengths $\lambda$, oscillator strengths $f$ and radiative transition probabilities $A_r$ have been calculated using the SUPERSTRUCTURE code developed at UC London [14], which uses a multi-configuration expansion of the wave functions. The atomic Hamiltonian includes most of the Breit Pauli relativistic corrections (one-body and two-body terms). The non-relativistic and relativistic eigenstates are obtained by diagonalizing the Schrödinger and Breit Pauli Hamiltonian respectively. The matrix transformation between both eigenstates is then used to transform non-relativistic autoionization transition matrix elements to fine-structure autoionization probabilities $A_a$, in the AUTOLJS code [15]. The radial parts of the one electron wave-functions are calculated in scaled Thomas-Fermi-Dirac potentials, the scaling parameters, for each $l$ orbital, being derived by minimizing the energies of some selected
3.2 Results

Calculations have been done for 11 ions from $\text{Fe}^{+16}$ to $\text{Fe}^{+6}$ using the ground state configuration and the excited configurations accessible by absorption (i.e., by electric-dipole transitions). For example:

$\text{Fe}^{+16}$: $1s^22s^22p^6$, $1s^22s^22p^53s$, $1s^22s^22p^53d$, $1s^22s^22p^54s$, $1s^22s^22p^54d$, $1s^22s2p^64p$

and

$\text{Fe}^{+6}$: $1s^22s^22p^63s^23p^63d^2$, $1s^22s^22p^53s^23p^63d^3$, $1s^22s^22p^53s^23p^63d^24s$, $1s^22s^22p^53s^23p^63d^24d$, $1s^22s2p^63s^23p^63d^24p$.

For $\text{Fe}^{+16}$, the excited configurations give bound states. Whereas for $\text{Fe}^{+15}$ to $\text{Fe}^{+6}$, the excited configurations correspond to autoionizing states. As examples we provide in Tables 2, 3, the wavelengths, absorption oscillator strengths, radiative and autoionization probabilities for $\text{Fe}^{+15}$, $\text{Fe}^{+14}$ and $\text{Fe}^{+8}$. One can observe the dramatic increase in the autoionization probabilities from $\text{Fe}^{+15}$ to $\text{Fe}^{+8}$. Moreover, the number of possible autoionizing channels increases also dramatically. This, in particular, explains why one does not observe the emission lines in Seyfert 2 which could correspond to the absorption lines in Seyfert 1 (see Fig. 2). That is, for L-lines, the photo-excited bound states, $\text{Fe}^{+23}$ to $\text{Fe}^{+16}$, decay by the reverse radiative transition whereas the photo-excited autoionizing states, $\text{Fe}^{+15}$ to $\text{Fe}^{+6}$, decay preferentially by autoionization.
4 Synthetic spectral modeling for the iron inner-shell photo-excitation lines

The optical depth $\tau_{ij}(\nu)$ due to an absorption line ($i \rightarrow j$) can be written as

$$\tau_{ij}(\nu) = N_{\text{ion}} \times \sigma_{ij}(\nu)$$

where $N_{\text{ion}}$ is the ionic column density along the line of sight to the source (in cm$^{-2}$) and $\sigma_{ij}(\nu)$ is the photo-excitation cross-section from $i$ to $j$.

The photo-excitation (or photo-absorption) cross-section is:

$$\sigma_{ij}(\nu) = \frac{\pi e^2}{m_e c} f_{ij} \phi(\nu)\phi(\nu), \quad (1)$$

where $e$ and $m_e$ are the electron charge and mass, $c$ is the speed of light, $f_{ij}$ the absorption oscillator strength, and $\phi(\nu)$ is a normalized line profile.

In Fig 5, the relative photo-absorption cross-sections of Fe$^{+16}$ to Fe$^{+6}$ are presented with the normalization factor being the same for each graph. If instrumental width is the dominant broadening process of the lines, the same gaussian profile can be used for all lines. The graph in the lower right is the sum of all the contributions with the assumption that each ion has the same abundance.

5 Conclusion

The new generation of X-ray satellites (*Chandra* and XMM-Newton) provide us with higher resolution spectra than was previously available. For the first time, we have access to high resolution X-ray spectroscopy of non-solar objects.
In particular, observations of Seyfert 1 galaxies, show very complex spectra with the presence of numerous absorption lines. Accurate atomic data are crucial to infer most of the physical and geometrical parameters of the “Warm Absorber”. We have calculated complete atomic data sets (wavelength, oscillator strength, auto-ionization rates) for inner-shell n=2-3 and n=2-4 (mainly 2p–3d, 2p–4d) photo-excitation for Fe ions (from 10 electrons to 20 electrons). Observations in UV, visible and infra-red wavelengths, where those Fe ions emit the most, are also important to have a realistic plasma modeling.

References

[1] Gabriel AH, Jordan C MNRAS 1969;145:241.
[2] Bely-Dubau F, Dubau J, Faucher P, Gabriel AH MNRAS 1982;198:239.
[3] Porquet D, Dubau J A&AS 2000;143:495.
[4] Porquet D, Mewe R, Dubau J, Raassen AJJ, Kaastra JS A&A 2001;376:1132.
[5] Sako M, Kahn SM, Behar E, Kaastra JS, et al. A&A 2001;365:L168.
[6] Blustin AJ, Branduardi-Raymont G, Behar E, et al. KC A&A 2002;392:453.
[7] Kaspi S, Brandt WN, George IM, et al. ApJ 2002;574:643.
[8] Kinkhabwala A., Sako M., Behar E. et al. ApJ 2002;575:732.
[9] Behar E, Sako M, Kahn SM ApJ 2001;563:497.
[10] Seyfert CK ApJ 1943;97:28.
[11] Antonucci RRJ, Miller JS. ApJ 1985;297:621.
[12] Urry CM, Padovani P PASP 1995;107:803.
[13] Halpern JP ApJ 1984;281:90.

[14] Eissner W, Jones M, Nussbaumer H Comp Phys Commun 1974;8:270.

[15] TFR Group, Dubau J, Loulergue M J Phys B 1981;15:1007.
Table 1
Energy (keV) and wavelength (Å) ranges, as well as the spectral resolution of the spectrometers aboard the new generation of X-ray satellites: *Chandra* (NASA) and *XMM-Newton* (ESA). The LETG and the HETG are onboard *Chandra*, and the RGS is on board *XMM-Newton*.

|         | LETG     | HETG     | RGS      |
|---------|----------|----------|----------|
| E (keV) | [0.07 – 8.86] | [0.4 – 10.0] | [0.35 – 2.5] |
| λ (Å)   | [1.4 – 170] | [1.2 – 31] | [5 – 38] |
| Δλ (Å)  | 0.05     | 0.012-0.023 | 0.06     |
Table 2
Absorption oscillator strengths, wavelengths, radiative and autoionization probabilities
(from the ground level of Fe$^{15+}$) 1s$^2$2s$^2$2p$^6$3s$^2$ 2$S_{1/2}$

| to the upper level | f (abs) | $A_r$(s$^{-1}$) | $\lambda$(Å) | $A_a$(s$^{-1}$) |
|--------------------|---------|----------------|---------------|----------------|
| 1s$^2$2s$^2$2p$^5$3s$^2$ 2$P_{3/2}$ | 0.07 | 7.96 (+11) | 17.20 | 8.50 (+12) |
| 1s$^2$2s$^2$2p$^5$3s$^2$ 2$P_{1/2}$ | 0.04 | 8.76 (+11) | 16.92 | 8.71 (+12) |
| 1s$^2$2s$^2$2p$^5$3s$^3$d 2$P_{3/2}$ | 0.06 | 8.74 (+11) | 15.44 | 1.95 (+12) |
| 1s$^2$2s$^2$2p$^5$3s$^3$d 4$D_{1/2}$ | 0.12 | 3.47 (+12) | 15.36 | 7.46 (+05) |
| 1s$^2$2s$^2$2p$^5$3s$^3$d 4$D_{3/2}$ | 0.22 | 3.08 (+12) | 15.34 | 4.04 (+10) |
| 1s$^2$2s$^2$2p$^5$3s$^3$d 2$D_{3/2}$ | 0.35 | 5.03 (+12) | 15.20 | 2.13 (+12) |
| 1s$^2$2s$^2$2p$^5$3s$^3$d 2$P_{1/2}$ | 0.94 | 2.75 (+13) | 15.09 | 4.40 (+12) |
| 1s$^2$2s$^2$2p$^5$3s$^3$d 2$P_{3/2}$ | 1.50 | 2.20 (+13) | 15.07 | 1.82 (+12) |
| 1s$^2$2s$^2$2p$^6$3s$^3$p 2$P_{1/2}$ | 0.08 | 2.87 (+12) | 13.96 | 5.87 (+13) |
| 1s$^2$2s$^2$2p$^6$3s$^3$p 2$P_{3/2}$ | 0.19 | 3.20 (+12) | 13.94 | 4.10 (+13) |
| 1s$^2$2s$^2$2p$^5$3s$^4$d 4$D_{1/2}$ | 0.12 | 5.11 (+12) | 12.48 | 1.32 (+12) |
| 1s$^2$2s$^2$2p$^5$3s$^4$d 2$P_{3/2}$ | 0.25 | 5.31 (+12) | 12.46 | 1.20 (+12) |
| 1s$^2$2s$^2$2p$^5$3s$^4$d 4$D_{3/2}$ | 0.29 | 6.38 (+12) | 12.33 | 1.49 (+12) |
| 1s$^2$2s$^2$2p$^5$3s$^4$d 2$P_{1/2}$ | 0.16 | 7.22 (+12) | 12.33 | 1.51 (+12) |
| 1s$^2$2s$^2$2p$^6$3s$^4$p 2$P_{3/2}$ | 0.05 | 1.35 (+12) | 11.19 | 5.60 (+11) |
| 1s$^2$2s$^2$2p$^6$3s$^4$p 2$P_{1/2}$ | 0.03 | 1.44 (+12) | 11.19 | 5.02 (+11) |
Table 3
Absorption oscillator strengths, wavelengths, radiative and autoionization probabilities
(from the ground level of Fe$^{14+}$) 1$s^22s^22p^63s^2 \, ^1S_0$

| to the upper level                  | f (abs) | $A_r$(s$^{-1}$) | $\lambda$(Å) | $A_a$(s$^{-1}$) |
|-------------------------------------|---------|-----------------|---------------|-----------------|
| 1$s^22s^22p^53s^23d \, ^3D_1$       | 0.59    | 5.49 (+12)      | 15.51         | 7.75 (+12)      |
| 1$s^22s^22p^53s^23d \, ^1P_1$       | 2.55    | 2.44 (+13)      | 15.26         | 1.43 (+13)      |
| 1$s^22s^2p^63s^23p \, ^1P_1$        | 0.27    | 3.05 (+12)      | 14.09         | 8.99 (+13)      |
| 1$s^22s^22p^53s^24d \, ^3D_1$       | 0.37    | 5.12 (+12)      | 12.74         | 8.49 (+12)      |
| 1$s^22s^22p^53s^24d \, ^1P_1$       | 0.41    | 5.80 (+12)      | 12.60         | 8.78 (+12)      |
| 1$s^22s^2p^63s^24p \, ^1P_1$        | 0.08    | 1.42 (+12)      | 11.38         | 8.82 (+13)      |

(from the ground of Fe$^{8+}$) 1$s^22s^22p^63s^23p^6 \, ^1S_0$

| to the upper level                  | f (abs) | $A_r$(s$^{-1}$) | $\lambda$(Å) | $A_a$(s$^{-1}$) |
|-------------------------------------|---------|-----------------|---------------|-----------------|
| 1$s^22s^22p^53s^23p^63d \, ^3D_1$   | 0.66    | 5.37 (+12)      | 16.59         | 4.19 (+14)      |
| 1$s^22s^22p^53s^23p^63d \, ^1P_1$   | 1.52    | 1.27 (+13)      | 16.33         | 4.77 (+14)      |
| 1$s^22s^22p^53s^23p^64d \, ^1P_1$   | 0.26    | 2.67 (+12)      | 14.59         | 4.05 (+14)      |
| 1$s^22s^22p^53s^23p^64d \, ^3D_1$   | 0.18    | 1.89 (+12)      | 14.39         | 4.00 (+14)      |
| 1$s^22s^2p^63s^23p^64p \, ^1P_1$    | 0.06    | 8.52 (+11)      | 12.80         | 6.20 (+13)      |
Fig. 1. The RGS (XMM-Newton) first order spectrum of Seyfert 1 IRAS 13349+2438 corrected for cosmological redshift ($z = 0.10764$), from Sako et al. [5]. The wavelength bins are approximately 0.1 Å wide. A best-fit model spectrum is superimposed in red.

Fig. 2. Effective-area-corrected, first-order (XMM/RGS 1 (red) and (XMM/RGS 2) (blue)) first-order spectra of Seyfert 2 NGC 1068 shifted to its rest frame ($z = 0.00379$), from Kinkhabwala et al. [8]. The spectral discontinuities are due to chip gaps in the CCD arrays, bad pixels, etc.

Fig. 3. Chandra/HETG spectrum of Seyfert 1 NGC 3783 binned to 0.01 Å focusing in the wavelength range [15-18 Å] from Kaspi et al. [7]. Broad absorption feature from blended inner-shell 2p3d absorption lines of Fe ions.

Fig. 4. A schematic diagram of the Unified Scheme of AGN, from Urry & Padovani [12]. Surrounding the central supermassif black hole is a luminous accretion disk. The so-called “Broad Line Region” and “Narrow Line Region” produces broad lines and narrow lines observed in the optical range. The contour of the “Warm Absorber” observed in X-ray is also shown, as well as, jets only seen in Radio-Loud objects.

Fig. 5. Photo-absorption cross-sections of the different Fe ions ($Fe^{+16}$ to $Fe^{+6}$) constituting the unresolved Fe-L feature, versus wavelengths. The final graph is built from the former graphs, assuming the same abundance for each ion.
Figure 1

IRAS 13349+2438
XMM-Newton/RGS

Photon cm$^{-2}$ s$^{-1}$ Å$^{-1}$

0 2×10$^{-4}$ 4×10$^{-4}$

10 15 20 25 30 35

wavelength (Å)

Ne X Lyα, Fe XX, (r), Fe XIX, Fe XVIII, Fe XVII, Fe VII – XII, O VIII Lyα, O VII Lyβ, N VII Lyα, N VII Lyβ, (4) XA, (4) IIA O, (4) IA, N IV Lyα, C IV Lyα, C III Lyα, C IV Lyβ, C IV He 7, C II Lyα, C
Figure 2
Figure 3

Flux [$\times 10^{-13}$ ergs cm$^{-2}$ s$^{-1}$ Å$^{-1}$]

Rest Wavelength [Å]

2p - 3d UTA

O Fe
Figure 4
Figure 5