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Atomic Physics Calculations for Iron L-line Spectra

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Abstract. Absorption L-lines of iron ions are observed, in spectra of Seyfert 1 galaxies by the new generation of X-ray satellites: Chandra and XMM-Newton. Lines associated to Fe^{23+} to Fe^{16+} have been already observed in emission, in the solar corona and in laboratory. Whereas, those corresponding to Fe^{15+} to Fe^{6+} have not been observed as emission lines, the upper level of the transition decaying preferentially by autoionization. Many atomic data are available for the first ion set. For the second set, some data have been recently published for n=2 to n'=3 transitions. We have recalculated them using another theoretical approach and have extended them to n'=4.

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 of Gabriel and Jordan (1969), have been extended from solar to non-solar coronae and also to photoionized plasmas by Porquet, Dubau (2000), Porquet et al. (2001). Besides these K-lines, Fe-L lines have also been observed in X-ray spectra, for Seyfert 1 (Sako et al. 2001, Blustin et al. 2002, Kaspi et al. 2002), and for Seyfert 2, (Kinkhabwala et al. 2002) 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 of Behar et al. (2001), 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, XMM (Bustin et al. 2002), and Chandra (Kaspi et al. 2002), show that the statistical assumption is not justified at least for this object : fine details 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, the use of a statistical width artificially increases the real width of the lines (Iglesias et al. 2003). We have therefore re-calculated all the atomic data of Behar et al. (2001) , extending them to n'= 4 transitions, giving a particular importance to the numerous possible autoionization channels (Dubau, Porquet, Zabaydullin, 2003).

2. Calculations of atomic parameters

2.1. Method

Wavelengths λ, oscillator strengths f and radiative transition probabilities A_r have been calculated using the SUPERSTRUCTURE code (Eissner et al. 1974) 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 eigen-states is then used to transform non-relativistic autoionization transition matrix elements to fine- structure autoionization probabilities A_a, in the AUTOLSJ code, (TFR Group, Dubau, Loulergue 1981). 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 LS terms.

2.2. Results

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

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 Fe^{23+} to Fe^{16+}, the excited configurations give bound states. Whereas for Fe^{+15} to Fe^{+6}, the excited configurations correspond to autoionizing states. As example, we provide in Table 1, the wavelengths, absorption oscillator strengths radiative and autoionization probabilities for Fe^{14+} and Fe^{8+}. One can observe the dramatic increase in the autoionization probabilities from Fe^{14+} to Fe^{8+}.

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Moreover, the number of possible autoionizing channels increases also. In particular, this explains why one does not observe the emission lines in Seyfert 2 which could correspond to the absorption lines in Seyfert 1. That is, for L-lines, the photo-excited bound states, Fe^{23+} to Fe^{16+}, decay by the reverse radiative transition whereas the photo-excited autoionizing states, Fe^{15+} to Fe^{6+}, decay preferentially by autoionization.

Table 1. Absorption oscillator strengths, wavelengths, radiative and autoionization probabilities

(from the ground level of Fe^{14+}) to the upper level)	$1s^2 2s^2 2p^6 3s^2\ {}^1S_0$ f (abs)	$A_r(s^{-1})$	λ(Å)	$A_a(s^{-1})$
$1s^2 2s^2 2p^5 3s^2 3d\ {}^3D_1$	0.59	5.49 (+12)	15.51	7.75 (+12)
$1s^2 2s^2 2p^5 3s^2 3d\ {}^1P_1$	2.55	2.44 (+13)	15.26	1.43 (+13)
$1s^2 2s 2p^6 3s^2 3p\ {}^1P_1$	0.27	3.05 (+12)	14.09	8.99 (+13)
$1s^2 2s^2 2p^5 3s^2 4d\ {}^3D_1$	0.37	5.12 (+12)	12.74	8.49 (+12)
$1s^2 2s^2 2p^5 3s^2 4d\ {}^1P_1$	0.41	5.80 (+12)	12.60	8.78 (+12)
$1s^2 2s 2p^6 3s^2 4p\ {}^1P_1$	0.08	1.42 (+12)	11.38	8.82 (+13)
(from the ground of Fe^{8+}) to the upper level)	$1s^2 2s^2 2p^6 3s^2 3p^6\ {}^1S_0$ f (abs)	$A_r(s^{-1})$	λ(Å)	$A_a(s^{-1})$
$1s^2 2s^2 2p^5 3s^2 3p^6 3d\ {}^3D_1$	0.66	5.37 (+12)	16.59	4.19 (+14)
$1s^2 2s^2 2p^5 3s^2 3p^6 3d\ {}^1P_1$	1.52	1.27 (+13)	16.33	4.77 (+14)
$1s^2 2s^2 2p^5 3s^2 3p^6 4d\ {}^1P_1$	0.26	2.67 (+12)	14.59	4.05 (+14)
$1s^2 2s^2 2p^5 3s^2 3p^6 4d\ {}^3D_1$	0.18	1.89 (+12)	14.39	4.00 (+14)
$1s^2 2s 2p^6 3s^2 3p^6 4p\ {}^1P_1$	0.06	8.52 (+11)	12.80	6.20 (+13)

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