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THEORETICAL SPECTRA OF Fe XXIII - Fe XIX IONS IN TWO CALCULATION METHODS

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Résumé :

Deux méthodes de calcul des paramètres atomiques nécessaires à l'analyse du spectre X des ions du Fe XXIII - Fe XIX (1.85 - 2 Å) sont comparées. La comparaison est faite sur les raies satellites dielectroniques du type $1s2s^k2p^n - 1s^22s^k2p^{n-1}$ (longueurs d'onde, probabilités de transition radiative et d'autoionisation, facteurs de raies). Cette étude a pour but l'interprétation des spectres X émis par les plasmas chauds et de faible densité (éruptions solaires et plasmas de Tokamak).

Abstract :

Two different calculation methods are compared for Fe XXIII - Fe XIX spectra in the X-ray range between 1.85 - 2 Å, for transitions of the type $1s2s^k2p^n - 1s^22s^k2p^{n-1}$. Wavelengths, radiative transition and autoionization probabilities as well as the intensity factors are compared. These parameters are given in order to diagnosis low density plasmas as found in solar flares and Tokamak devices.

The X-ray emission of highly ionized atoms in low density, hot plasmas such as observed in solar flares or Tokamak devices is dominated by the resonance line emission of the H and He-like ions and their associated dielectronic satellites. The analysis of these satellite lines is of fundamental importance for the investigation of the physics of the highly ionized ions as well as for the interpretation in term of temperature and density diagnostics of the emitting plasmas. The most prominent satellite lines observed correspond to the transitions $2s2p-1s2s$, $2p^2-1s2p$, $1s2s2p-1s^22s$, $1s2p^2-1s^22p$. That is the reason why the autoionization states of two and three electron systems have been the most well-studied in the past (1). On the contrary, for autoionization states with four or more electrons, there are only few observations (2, 3), few calculations and practically no comparison. This is due to the complexity of the theoretical problem as well as the observational one. We present here a comparison between two different methods : the MZ method by Vainstein and Safronova (4) and the AUTOLSJ method by Dubau et al. (5). The comparison is done on Fe XXIII - Fe XIX for transitions of the type $1s2s^k2p^n - 1s^22s^k2p^{n-1}$. Iron was chosen due to the possibility of comparison with observations.

1) Calculation methods

A common feature of both methods is that the energy matrix is constructed on the basis of the L-S scheme and the relativistic corrections are included within the framework of the Breit-Pauli operator. The methods use a perturbational approach. The main difference is in the choice of the mono-electronic wave functions used for building the unperturbed wave functions of the n-electron system. In the MZ method these mono-electronic wave functions are hydrogenic whereas in the SUPERSTRUCTURE program (14) used by AUTOLSJ, the wave functions are calculated in a scaled Thomas Fermi Dirac potential, the scaling parameters are obtained by a self consistent energy minimization procedure. Another difference appears on the basis size of the unperturbed wave functions. In the MZ method, the basis is complete including both bound and continuum states when in SUPERSTRUCTURE the truncated basis is limited to the most important bound states, the apparent restriction can be compensated by the minimization procedure. In the MZ method the energy of a given state is calculated by diagonalization procedure of the energy matrix elements between the states of the same Laser complex, the contribution of all states belonging to the other complexes is introduced as a second order perturbation correction.

In the SUPERSTRUCTURE program the diagonalization is done for all the states of the truncated basis. The MZ method is better for systems with few electrons since the hydrogenic orbitals are realistic and the method can be carried to any order of perturbation on a complete basis. For systems with many electrons and an average potential being more realistic, SUPERSTRUCTURE can give accurate results faster than MZ which becomes rapidly untractable.

As mentioned above, in both approximations the relativistic corrections were taken into account within the framework of the Breit Pauli operator. There are the one-body operators as mass, Darwin and spin-orbit and the two-body operators as spin-spin contact, two-body Darwin, orbit-orbit, spin-other orbit and spin-spin.

In both methods each of the operators is calculated with non relativistic functions. The radiative probabilities A_r and the autoionization probabilities A_a are calculated in both schemes with the use of the vector coupling coefficients obtained upon diagonalization of the matrix energy (in MZ with the complex state set and in AUTOLSJ with the truncated basis set).

In the following sections we compare the wavelengths λ , the radiative transitions probabilities A_r and the line factor Q_d defined as :

$$Q_d = (2J + 1) \frac{A_a A_r}{\Sigma A_a + \Sigma A_r}$$

where ΣA_r is the total radiative probability and ΣA_a the total autoionization probability for the upper level of the transition.

2) Results

For each ion a selection of the strongest lines is given in the table. As far

Table : Dielectronic satellite lines ($n = 2$) calculated with AUTOLSJ method (a) and MZ method (b)

	λ (Å)		A_r (10^{13} s^{-1})		Q_d (10^{13} s^{-1})	
	(a)	(b)	(a)	(b)	(a)	(b)
<u>$1s2s2p^2 - 1s^22s^2p$ (Fe XXIII)</u>						
$^3D_3 - ^3P_2$	1.8721	1.8754	22.2	23.1	58.8	66.2
$^3D_3 - ^3P_1$	1.8699	1.8731	32.4	31.7	38.2	48.1
$^3P_1 - ^3P_1$	1.8637	1.8721	26.1	24.2	17.6	17.3
<u>$1s2s^22p^2 - 1s^22s^22p$ (Fe XXII)</u>						
$^2D_{3/2} - ^2P_{1/2}$	1.8789	1.8821	29.2	30.4	20.5	25.1
$^2D_{3/2} - ^2P_{3/2}$	1.8814	1.8849	19.7	20.5	27.4	33.4
$^2P_{3/2} - ^2P_{3/2}$	1.8780	1.8814	57.7	56.9	8.4	12.0
<u>$1s2s^22p^3 - 1s^22s^22p^2$ (Fe XXI)</u>						
$^3D_1 - ^3P_0$	1.8908	1.8943	26.7	29.5	15.1	18.6
$^3D_2 - ^3P_1$	1.8929	1.8965	20.3	22.1	20.3	25.2
$^3P_2 - ^3P_2$	1.8896	1.8931	30.8	32.8	9.3	11.5
<u>$1s2s^22p^4 - 1s^22s^22p^3$ (Fe XX)</u>						
$^4P_{3/2} - ^4S_{3/2}$	1.9054	1.9082	19.4	20.2	6.4	7.4
$^2D_{3/2} - ^2D_{3/2}$	1.9030	1.9057	46.6	47.8	1.2	1.8
$^2P_{3/2} - ^2D_{3/2}$	1.9007	1.9036	44.8	44.5	3.2	3.5
<u>$1s2s^22p^5 - 1s^22s^22p^4$ (Fe XIX)</u>						
$^3P_2 - ^3P_2$	1.9157	1.9174	28.9	29.4		
$^3P_0 - ^3P_1$	1.9145	1.9159	42.9	43.4		
$^1P_1 - ^1S_0$	1.9140	1.9160	63.7	63.3		

as we are concerned with low density plasmas we give only the Q_d factor corresponding to dielectronic recombination on the ground level of the recombining ion (FeXXI, FeXX).

For FeXIX there is no population process by dielectronic recombination from the lowest level $1s^2 2s^2 2p^3 \ ^4S_{3/2}$ of FeXX. For this ion we give only the wavelengths and radiative probabilities.

One can see on the table that there is a systematic difference of $\sim 0.003 \text{ \AA}$ on the wavelengths. This difference seems to decrease for FeXX that is when the number of electrons is growing up. This tendency can be explained by the fact that for system with many electrons an average potential is more realistic.

For the two other parameters A_r and Q_d the agreement between the two methods is quite good for large values of these parameters. More important discrepancies appear when these values are smaller. The full set of data will be published later in J. Phys. B.

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