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Calculations of Atomic Parameters of Highly Charged Fe Ions for Interpreting Astrophysical Spectra

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ABSTRACT

Study of physical processes in astrophysical and fusion plasmas consists of detail analysis of high resolution atomic spectra obtained from such plasmas. The X-ray spectra from iron K-shell and L-shell ions are particularly important for astrophysics as they are in wavelength range covered by telescopes on board space observatories like Chandra and XMM-Newton. To conduct the astrophysical plasma diagnostic studies of Active galactic nuclei (AGN), solar corona and other similar astronomical entities, a large number of accurate transition data both from theory and experiment are indispensable. Here we have calculated similar atomic data in use for these studies by multi-configuration Dirac-Fock (MCDF) formalism used in Grasp2K code. Calculations consists of ground and few low level excited states in He-like and Li-like Fe ions and some important transitions connecting these levels.

Keywords: *Astrophysics; Atomic Data; Plasma Diagnostics.*

1.0 Introduction

High-resolution X-ray spectra's are obtained by Chandra X-ray Observatory and X-ray Multi-Mirror Mission (XMM-Newton) in the past, and also by Astrosat and Astro-H launched recently by ISRO and JAXA respectively. Spectra obtained by these observatories over the year have shown the presence of highly-charged ions in a variety of non-terrestrial sources such as corona of the Sun, stellar atmosphere, cluster of galaxies and super-nova remnants.

These sources have temperatures greater than 1 million Kelvin and which results in the production of highly charged Fe ions, and the radiation emitted at such temperatures falls in the X-ray region. All these astrophysical observations put new demands on atomic data, including line positions, excitation cross sections, radiative rates and oscillator strengths of most abundant highly charged ions like those of iron.

To address these needs there are worldwide efforts both in experimentally and theoretically, to identify the unknown lines and their proper assignments to their respective charge states in-order to have a complete and reliable atomic data.

Past experimental work consist of data obtained at Lawrence Livermore National Laboratory (LLNL) Electron Beam Ion trap (EBIT).

There is a line identification work done by Seely et at (1986) [1] in solar flare spectra, and the laboratory measurements by Beiersdorfer et al. (1989, 1993) [2-3], Decaux & Beiersdorfer et al. (1993) [4] and Decaux et al. (1995, 1997) [5-6]. Still the K-vacancy level structures of Fe ions were not fully identified till the critical complilation of Shirai et al. (2000) [7] followed. Later extensive work on radiative and auger rates in Fe XXV – Fe XXI was carried out by Chen (1986) [8] and Kato et al. (1997) [9], which in fact provided some reliable data in the above field.

In an important theoretical work, done by Palmeri et al. (2002) [10] have shown that the K-threshold resonance behavior is dominated by radiation and auger damping which include a smeared edge. Spectator Auger decay, the main contributor of the K-resonance width, was completely ignored in

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most of the previous close-coupling calculations of high-energy continuum processes in Fe ions by Berrington et al. (1997) [11], Donnelly et al. (2000) [12], Berrington & Ballance (2001) [13] and Balance et al. (2001) [14].

The present work is intended to report the atomic data for Fe K-shell spectra which consists of Fe XXV and Fe XXIV i.e. He-like and Li-like Fe by Grasp2k calculations [15-18]. Grasp2k calculations have an edge over other calculations like those performed by COWAN code, R-matrix and close coupling because these are completely *ab-initio* in nature. Moreover, it is based on multi-configuration Dirac-Fock (MCDF) method developed by Grant and co-workers [19] and most importantly the relativistic corrections like transverse energy photons, vacuum polarization effect and self-energy can be calculated by this code.

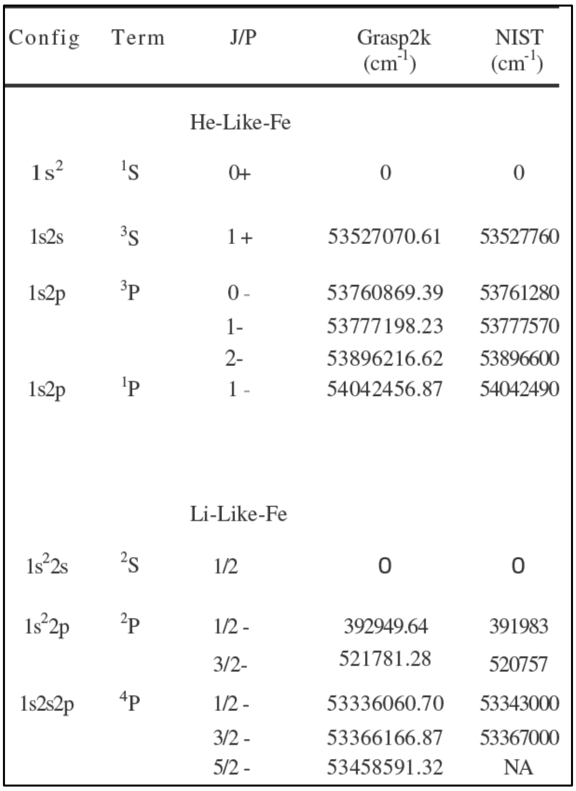
2.0 Theoretical Background of MCDF Calculations

As Fe XXV and Fe XXIV are highly charged ions, it is very important to include the relativistic and correlation effects in the calculations of ground level as well as of low lying excited levels. MCDF approach is best suited for such sophisticated calculations due to its *ab-initio* nature, which in principle is applicable to any atomic system from negative to highly positively charged ions. In this approach an atomic state is approximated by the superposition of the configuration state function (CSFs) of the same symmetry.

$$\Psi_\alpha = \sum_{r=1}^{n} c_r(\alpha) | Y_r PJM >$$

In above equation the complete atomic state function Ψ_α has been written as a linear combination of all the possible configuration state functions. In Grasp2k code this basis function is systematically enlarged by active space method [20] to capture most of the correlation and relativistic effects. The CSFs are basically the anti-symmetries product of a common set of ortho normal orbital which are optimized self-consistently on the basis of the Dirac-Coulomb Hamiltonian. Further the relativistic corrections to the electron-electron interaction are added in a second step by diagonal the Dirac-Coulomb-Breit Hamiltonian matrix.

Table 1: Excitation Energy Levels of $1s^2$ Ground and 1s2s, 1s2p Excited State Configuration of He-Like Fe And Energy Levels of $1s^22s$ Ground and $1s^22p$, 1s2s2p Excited State Configuration of Li-Like Fe.

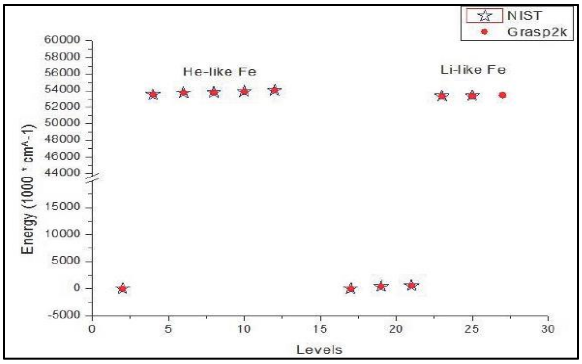


Config	Term	J/P	Grasp2k (cm^{-1})	NIST (cm^{-1})
		He-Like-Fe		
$1s^2$	^1S	0+	0	0
1s2s	^3S	1 +	53527070.61	53527760
1s2p	^3P	0 -	53760869.39	53761280
		1-	53777198.23	53777570
		2-	53896216.62	53896600
1s2p	^1P	1 -	54042456.87	54042490
		Li-Like-Fe		
$1s^22s$	^2S	1/2	0	0
$1s^22p$	^2P	1/2 -	392949.64	391983
		3/2-	521781.28	520757
1s2s2p	^4P	1/2 -	53336060.70	53343000
		3/2 -	53366166.87	53367000
		5/2 -	53458591.32	NA

3.0 Computational Details

To work on He-like system we have first generated spectroscopic orbitals for ($1s^2$ + 1s2s) configurations simultaneously and then for 1s2p excited state configurations and in case of Li-like system similar procedure is followed for $1s^22s$ as ground state configuration and $1s^22p$, 1s2s2p for excited state configurations. After successful generation of spectroscopic orbitals for both the ions we added 2l and 3l correlation layers of valid approximation by first doing single-double (SD) excitations to first 2l level, then to 3l level [20]. While applying such SD approximation, all the newly generated orbitals are made orthogonal to others of the same symmetry. The initial shapes of radial orbitals were obtained in Thomas-Fermi potential and for virtual orbitals screened hydrogenic potential is used. Once all the radial orbitals are obtained they all are made to converge by keeping self-consistency threshold set to 10^{-7} s^{-1}. All radial orbital are separately optimized for each of the two atomic states of interest. After adding the required configuration in the last step by using RCI-routine of Grasp2k code relativistic corrections along with self-energy term and vacuum polarisation are added to get more accurate energy levels and there by better transition rates data. Having done all this, our energy levels for both He-like and Li-like systems are coming very close to the NIST atomic energy levels.

Fig 1: A comparison of the present computed Energy levels with NIST Databas.



4.0 Results and Discussion

4.1 Energy levels

Our results are listed in **Table 1**, where we have presented our calculated the level energies of He-like and Li-like Fe. It may be pointed out once again that the $1s^2$ state is used here as the ground state configuration and 1s2s, 1s2p as excited state configurations are used for He-like Fe ions, whereas for Li-like Fe ions $1s^22s$ is used as the ground and $1s^22p$, 1s2s2p as excited states configurations. We now compare our results of the level energies with those of NIST database [7] in **Fig 1**. It may here be pointed out that the NIST energy levels were extrapolated using experiments and COWAN code. As we can see, nearly all the computed values of ours are in good agreement with the NIST compilation; the two nearly overlap except at one point in Li-like system. In fact this level i.e. $^4P_{5/2-}$ belonging to 1s2s2p configuration is not even listed in NIST database. Remembering that Li-like ions of all the cosmically abundant elements like Fe, Ni and Cu etc. are actually used in astrophysical plasma diagnostic studies of active galactic nuclei or Solar corona, the presence of above noted level in our estimate turns out to be significant addition to the existing knowledge. It may here be pointed out that exclusion of an important level such as $^4P_{5/2}$ will adversely affect the plasma diagnostic studies while calculating the electron temperature G (T_e) and electron number density R(n_e). Where, G (T_e) is calculated as the ratio of forbidden plus inter-combination to the resonance and R (n_e) as the ratio of forbidden to the inter-combination transitions. Such transitions in highly charged ions take place between the ground levels and low lying excited levels. Thus if any of the level is not included in the atomic database it will have a huge adverse impact on the presently ongoing plasma diagnostic research for astrophysical plasma. Considering the importance of including one additional energy level $^4P_{5/2}$ in the existing NIST database, which makes it complete, we report all the important radiative transition rates for both the ions under study.

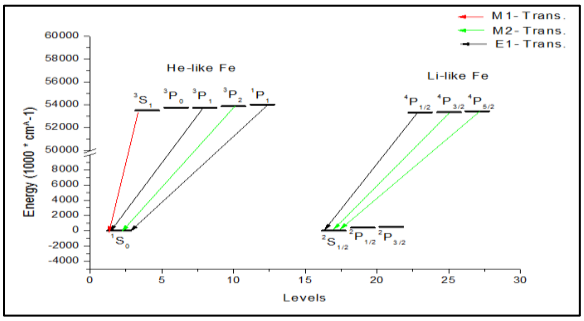
Table 2: Important radiative rate transitions (M1, M2 and E1) in He-Like and Li-Like Fe ion.

Upper Level	Lower Level	E_{cal} (keV)	E_{cal} (Kays)	A_{ij} (s^{-1})
		He-Like-Fe		
$^3S_1$[M1]	$^1S_0$	6.63	53527070.78	2.04×10^8
$^3P_2$[M2]	$^1S_0$	6.68	53896216.79	6.49×10^9
$^3P_1$[E1]	$^1S_0$	6.66	53777198.40	4.42×10^{13}
$^1P_1$[E1]	$^1S_0$	6.70	54042457.04	4.58×10^{14}
		Li-Like-Fe		
$^4P_{3/2}$[M2]	$^2S_{1/2}$	6.61	53366167.04	7.03×10^8
$^4P_{5/2}$[M2]	$^2S_{1/2}$	6.62	53458591.49	6.14×10^9
$^4P_{1/2}$[E1]	$^2S_{1/2}$	6.61	53336060.87	5.20×10^{12}

4.1 Radioactive rates

Results of estimate of radioactive rates are listed in **Table 2**, where important transition rates of He-like and Li-like Fe ions have been presented; the pictorial representation of transitions connecting the energy levels is shown as well in Figure 2. Special emphasis is given on computations of forbidden and inter-combination transitions in both the ions due to their use in astrophysical plasma diagnostic studies. It is very difficult to resolve these lines in laboratory experiments and this can also be inferred from the above table where nearly all the transitions in He-Like and Li-Like Fe lie in the 6.61 keV to 6.70 keV range. Obviously experimentalists would be highly benefited if the theoretical calculations of these lines are made available to them. In our calculations the focus is on the following three transitions which are of astrophysical importance i.e., two He-like $1s2p\ ^3P_2 \rightarrow 1s^2\ ^1S_0$ (M2-transition) and $1s2s\ ^3S_1 \rightarrow 1s^2\ ^1S_0$ (M1-transition) and one Li-like $1s2s2p\ ^4P_{5/2} \rightarrow 1s^22s\ ^2S_0$ (M2-transition). As expected the forbidden transitions $1s2p\ ^3P_2 \rightarrow 1s^2\ ^1S_0$ and $1s2s\ ^3S_1 \rightarrow 1s^2\ ^1S_0$ in He-Like Fe have low intensities compared to the allowed transition from $1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0$. This is also be confirmed from our transition rate calculations by Grasp2k. For example, if we compare our estimated allowed and forbidden transitions in He-like system, we can see that A_{ij} value for the forbidden transitions i.e. $1s2p\ ^3P_2 \rightarrow 1s^2\ ^1S_0$ and $1s2s\ ^3S_1 \rightarrow 1s^2\ ^1S_0$ are 6.49×10^9 and 2.04×10^8 respectively (see **Table 2)**, whereas in case of E1 allowed transition $1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0$ the transition rates turns out to be 4.58×10^{14}. And this is the primary reason why such astrophysically important forbidden transtions are not fully resolved from the intense allowed transitions even in beam foil spectroscopy experiments. All these experimental constraints in measuring such weak and near-by-occuring forbidden and intercombination transitions makes our theoretical computations of these transitions even more relevant for future identification work.

Fig 2: Radioactive Rate Transitions From Upper Excited Levels to Ground Level in He-Like and Li-Like Fe



5.0 Conclusions

Using fully relativistic Dirac-Fock formalism a new set of level energies, transition probabilities has been obtained for He-Like and Li-Like Fe which are of astrophysical importance. The presently computed data agrees well with the NIST computed database. However most of the reported energy levels in NIST for both the ions are experimentally extrapolated values done with COWAN code computations. Our values happens to be more reliable as it is fully relativistic in nature unlike COWAN code's pseudo-relativistic framework.

In these calculations most of the relativistic and correlation effects like transverse energy photon, vacuum polarization and self-energy corrections are included. Moreover, we are able to improve upon the NIST database by including one additional energy level, which may play important role in plasma diagnostics. We have put special emphasis on calculating the forbidden transitions, as they are the experimental indicators of the meta stable states present in the plasma. Presently revised atomic data for Fe^{24+} and Fe^{23+} is generated, which we feel is better equipped for reliable plasma diagnostics of Active galactic nuclei (AGN), solar corona and other similar astronomical bodies. We have also underlined the importance of calculating the forbidden lines, which would be a big help to experimentalists in many cases.

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